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

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Overview of Invited Talks and Sessions

(Lecture rooms C 130, C 230, C 243, C 264, and PC 203; Poster A, B, and C)

Invited Talks

CPP 3.1	Mon	9:30–10:00	C 243	**Time-resolved in-situ x-ray scattering to resolve structure formation in thin film processing** — •Eva M. Herzig
CPP 4.8	Mon	11:15–11:45	C 264	**Reconfigurable colloidal structures** — •Daniela J. Kraft
CPP 5.1	Mon	9:30–10:00	PC 203	**Strain-controlled criticality governs the nonlinear mechanics of fibre networks** — •Abhinav Sharma, Albert Licup, Karin Jansen, Robbie Rens, Michael Sheinman, Jordan Shivers, Jingchen Feng, Gijsje Koenderink, Fred MacKintosh
CPP 23.1	Tue	9:30–10:00	C 243	**Non-fullerene acceptors for commercially viable organic photovoltaics** — •Derya Baran
CPP 25.1	Tue	9:30–10:00	PC 203	**Understanding self-assembly in gyroid terpolymer films** — •Ilja Gunkel
CPP 25.6	Tue	11:15–11:45	PC 203	**Soft Interfaces Studied with the Quartz Crystal Microbalance** — •Diethelm Johannsmann, Arne Langhoff
CPP 30.1	Tue	11:45–12:15	C 264	**Novel hyphenated rheology techniques for the study of quiescent and flow-induced polymer crystallization** — Volker Räntzsch, Mürüvvet Begüm Özen, Karl-Friedrich Ratzsch, Gisela Guthausen, •Manfred Wilhelm
CPP 31.1	Tue	14:00–14:30	PC 203	**The role of correlations in the collective behaviour of microswimmer suspensions** — •Alexander Morozov
CPP 38.1	Wed	9:30–10:00	C 230	**The favorite polymer libations** — •Carlos M. Marques, Debashish Mukherji, Kurt Kremer
CPP 39.1	Wed	9:30–10:00	C 243	**Charge generation and recombination in an organic BHJ solar cell with low energetic offsets** — •Thuc-Quyen Nguyen
CPP 40.1	Wed	9:30–10:00	C 264	**Slippage over superhydrophobic surfaces: fundamentals and local phenomena** — •Clarissa Schönecker, David Schäffel, Kaloian Koynov, Doris Vollmer, Hans-Jürgen Butt
CPP 45.1	Wed	11:00–11:30	C 243	**Double-Semidilute Liquid and Gel Coacervates formed by Oppositely Charged Polyelectrolytes** — •Michael Rubinstein, Sergey Panyukov, Qi Liao
CPP 70.1	Thu	15:00–15:30	C 230	**Crystallization in melts of semi-flexible hard polymer chains: An interplay of entropies and dimensions** — •Wolfgang Paul, Timur Shakirov
CPP 72.1	Thu	15:00–15:30	C 264	**Ionic (in)homogeneity in metal-halide perovskites** — •Eva Unger
CPP 77.1	Fri	9:30–10:00	C 243	**High-Performance Organic Transistors** — •Karl Leo

Invited talks of the joint symposium SYMS

See SYMS for the full program of the symposium.

SYMS 1.1	Mon	15:00–15:30	H 0105	**Stochastic numerical algorithms: from molecular dynamics to big data analytics** — •Benedict Leimkuhler
SYMS 1.2	Mon	15:30–16:00	H 0105	**A Generally-Applicable Machine-Learning Scheme for Materials and Molecules** — •Michele Ceriotti

SYMS 1.3	Mon	16:00–16:30	H 0105	**Girsanov reweighting for path ensembles and Markov state models** — •Bettina G. Keller, Luca Donati, Carsten Hartmann
SYMS 1.4	Mon	16:45–17:15	H 0105	**Liquid State Theory Meets Deep Learning and Molecular Informatics** — •Alpha Lee
SYMS 1.5	Mon	17:15–17:45	H 0105	**Computational high-throuhgput screening of drug-membrane thermodynamics** — •Tristan Bereau

Invited talks of the joint symposium SYBS

See SYBS for the full program of the symposium.

SYBS 1.1	Tue	9:30–10:00	H 0105	**Bacterial collective behaviours** — •Knut Drescher
SYBS 1.2	Tue	10:00–10:30	H 0105	**Nonlinear dynamics of beating cilia and flagella: Swimming, steering, and synchronization** — •Benjamin M. Friedrich
SYBS 1.3	Tue	10:30–11:00	H 0105	**Learning to navigate in dynamic environments: animal behavior and artificial intelligence** — •Antonio Celani
SYBS 1.4	Tue	11:15–11:45	H 0105	**Suspensions of active colloids** — •Cecile Cottin-Bizonne, Félix Ginot, Isaac Theurkauff, Christophe Ybert
SYBS 1.5	Tue	11:45–12:15	H 0105	**Spontaneous chiral symmetry breaking in active fluids** — •Jörn Dunkel

Invited talks of the joint symposium SYVC

See SYVC for the full program of the symposium.

SYVC 1.1	Wed	15:00–15:30	H 0105	**Magneto-ionic control of interfacial magnetism** — •Geoffrey Beach
SYVC 1.2	Wed	15:30–16:00	H 0105	**Ionic Control of Materials Beyond Interfaces** — •Dustin Gilbert
SYVC 1.3	Wed	16:00–16:30	H 0105	**Microscopic Mechanisms of Memristive Switching in Metal Oxides** — •Rainer Waser, Stephan Menzel, Regina Dittmann
SYVC 1.4	Wed	17:00–17:30	H 0105	**In-situ and operando SQUID magnetometry under electrochemical control** — •Roland Würschum, Markus Gössler, Gregor Klinser, Eva-Maria Steyskal, Heinz Krenn
SYVC 1.5	Wed	17:30–18:00	H 0105	**Reversible chemistry as a tool for dynamic control of physical properties** — •Robert Kruk, Subho Dasgupta, Bijoy Das, Horst Hahn

Invited talks of the joint symposium SYTH

See SYTH for the full program of the symposium.

SYTH 1.1	Thu	9:30–10:00	H 0105	**Extracting the electrical properties of metal halide perovskite semiconductors using transient terahertz spectroscopy** — •Michael B. Johnston
SYTH 1.2	Thu	10:00–10:30	H 0105	**THz nanophotonics with 2D materials** — •Miriam SERENA Vitiello
SYTH 1.3	Thu	10:30–11:00	H 0105	**Nonlinear responses and 2D spectroscopy using THz electric and magnetic fields** — •Keith A Nelson
SYTH 1.4	Thu	11:15–11:45	H 0105	**Low energy electrodynamics of correlated spin systems.** — •N. Peter Armitage
SYTH 1.5	Thu	11:45–12:15	H 0105	**Lightwave scanning tunneling microscopy of single molecules** — Dominik Peller, Tyler L. Cocker, Ping Yu, Rupert Huber, •Jascha Repp

Invited talks of the joint symposium SYAM

See SYAM for the full program of the symposium.

SYAM 1.1	Fri	9:30–10:00	H 0105	**Bringing Dino-Birds to life – Synchrotron X-ray fluorescence and Raman imaging of ancient materials** — •Uwe Bergmann
SYAM 1.2	Fri	10:00–10:30	H 0105	**Linear and Nonlinear Optical Properties of Cultural Heritage Materials** — •Marta Castillejo
SYAM 1.3	Fri	10:30–11:00	H 0105	**Morphology and topology of multiscale pore networks: Imaging structural alteration and hydric invasion** — •Pierre Levitz

SYAM 1.4	Fri	11:15–11:45	H 0105	**Painting cracks: a way to reveal physical properties of matter** — •Ludovic Pauchard
SYAM 1.5	Fri	11:45–12:15	H 0105	**Finite element analysis and biomechanical interpretation of fossil material properties** — •Emily Rayfield

Sessions

CPP 1.1–1.11	Mon	9:30–13:00	C 130	**Focus: Molecularly Functionalized Low-Dimensional Systems I - organized by Antonio Setaro, Carola Meyer, Aravind Vijayaraghvan and Matteo Mannini**
CPP 2.1–2.6	Mon	9:30–11:00	C 230	**Electrical, Dielectrical and Optical Properties of Thin Films I**
CPP 3.1–3.12	Mon	9:30–13:00	C 243	**Organic Electronics and Photovoltaics - Layer Morphology and Molecular Aggregation**
CPP 4.1–4.13	Mon	9:30–13:00	C 264	**Complex Fluids and Colloids I (joint session CPP/DY)**
CPP 5.1–5.11	Mon	9:30–12:45	PC 203	**Polymer Networks and Elastomers I**
CPP 6.1–6.10	Mon	9:30–12:15	H 0112	**Magnetic nanoparticles (joint session MA/CPP)**
CPP 7.1–7.12	Mon	9:30–13:00	H 1058	**Biomaterials and Biopolymers (joint session BP/CPP)**
CPP 8.1–8.14	Mon	9:30–13:15	H 2032	**2D Materials (Symposium and Joint Session with HL and O): Session I (joint session DS/CPP/HL)**
CPP 9.1–9.12	Mon	10:00–13:15	BH-N 243	**Active Matter I (joint session DY/CPP/BP)**
CPP 10.1–10.10	Mon	10:30–13:00	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials I (joint session O/MM/DS/TT/CPP)**
CPP 11.1–11.7	Mon	11:15–13:00	C 230	**Responsive and Adaptive Systems**
CPP 12.1–12.8	Mon	15:00–17:30	C 130	**Focus: Molecularly Functionalized Low-Dimensional Systems II - organized by Antonio Setaro, Carola Meyer, Aravind Vijayaraghvan and Matteo Mannini**
CPP 13.1–13.6	Mon	15:00–16:30	C 243	**Organic Electronics and Photovoltaics - Hybrid and Organic Layer Systems**
CPP 14.1–14.10	Mon	15:00–17:45	C 264	**Interfaces and Thin Films I**
CPP 15.1–15.6	Mon	15:00–16:30	MA 144	**Solid-liquid interfaces: Reactions and electrochemisty I (joint session O/CPP)**
CPP 16.1–16.9	Mon	15:00–17:15	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials II (joint session O/MM/DS/TT/CPP)**
CPP 17.1–17.12	Mon	15:30–18:45	BH-N 243	**Active Matter II (joint session DY/CPP/BP)**
CPP 18.1–18.14	Mon	15:30–19:15	BH-N 334	**Focus: Droplets (joint session DY/CPP)**
CPP 19.1–19.6	Mon	16:45–18:15	MA 144	**Solid-liquid interfaces: Reactions and electrochemisty II (joint session O/CPP)**
CPP 20.1–20.62	Mon	17:30–19:30	Poster A	**Poster Session I**
CPP 21.1–21.12	Tue	9:30–13:00	C 130	**Focus: Smart Hydrogels and Hydrogel Based Devices I - organized by Gerald Gerlach, Walter Richtering and Thomas Hellweg**
CPP 22.1–22.4	Tue	9:30–10:30	C 230	**Data-driven Methods in Molecular Simulations of Soft-Matter Systems**
CPP 23.1–23.12	Tue	9:30–13:00	C 243	**Organic Photovoltaics I**
CPP 24.1–24.8	Tue	9:30–11:45	C 264	**Complex Fluids and Colloids II (joint session CPP/DY)**
CPP 25.1–25.11	Tue	9:30–13:00	PC 203	**Interfaces and Thin Films II**
CPP 26.1–26.14	Tue	9:30–13:15	H 2032	**2D Materials (Symposium and Joint Session with HL and O): Session II (joint session DS/CPP/HL)**
CPP 27.1–27.5	Tue	10:30–13:00	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials III (joint session O/MM/DS/TT/CPP)**
CPP 28.1–28.6	Tue	11:00–12:30	BH-N 334	**Condensed Matter Simulations augmented by Advanced Statistical Methodologies I (joint session DY/CPP)**
CPP 29.1–29.7	Tue	11:15–13:00	C 230	**Nanostructures, Nanostructuring and Nanosized Soft Matter I**
CPP 30.1–30.4	Tue	11:45–13:00	C 264	**Friction and Rheology**
CPP 31.1–31.7	Tue	14:00–16:00	PC 203	**Modeling and Simulation of Soft Matter I (joint session CPP/DY)**

CPP 32.1–32.13	Tue	14:00–16:00	Poster B	**Poster Session II**
CPP 33.1–33.42	Tue	14:00–16:00	Poster C	**Poster Session III**
CPP 34.1–34.5	Tue	14:00–15:15	BH-N 128	**Condensed Matter Simulations augmented by Advanced Statistical Methodologies II (joint session DY/CPP)**
CPP 35.1–35.7	Tue	14:00–15:45	BH-N 243	**Microswimmers I (joint session DY/BP/CPP)**
CPP 36.1–36.7	Tue	14:00–15:45	EB 107	**Particulate Matter: From microscopic interactions to collective motion (joint session DY/CPP)**
CPP 37.1–37.11	Wed	9:30–13:00	C 130	**Focus: Smart Hydrogels and Hydrogel Based Devices II - organized by Gerald Gerlach, Walter Richtering and Thomas Hellweg**
CPP 38.1–38.8	Wed	9:30–12:00	C 230	**Modeling and Simulation of Soft Matter II (joint session CPP/DY)**
CPP 39.1–39.4	Wed	9:30–10:45	C 243	**Organic Photovoltaics II**
CPP 40.1–40.12	Wed	9:30–13:00	C 264	**Wetting, Microfluidics and Confined Liquids I (joint session CPP/DY)**
CPP 41.1–41.11	Wed	9:30–12:15	MA 001	**Networks (joint session SOE/DY/BP) (joint session SOE/CPP/BP/DY)**
CPP 42.1–42.7	Wed	9:30–12:30	EMH 025	**Materials for Energy Storage I (joint session KFM/CPP)**
CPP 43.1–43.12	Wed	9:30–13:00	H 1028	**Membranes and Vesicles I (joint session BP/CPP)**
CPP 44.1–44.9	Wed	10:30–13:00	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials IV (joint session O/MM/DS/TT/CPP)**
CPP 45.1–45.7	Wed	11:00–13:00	C 243	**Charged Soft Matter, Polyelectrolytes and Ionic Liquids I**
CPP 46.1–46.58	Wed	11:00–13:00	Poster A	**Poster Session IV**
CPP 47.1–47.4	Wed	12:00–13:00	C 230	**Electrical, Dielectrical and Optical Properties of Thin Films II**
CPP 48.1–48.9	Wed	15:00–17:45	C 130	**Focus: Fundamental Physics of Perovskites I - organized by Lukas Schmidt-Mende and Vladimir Dyakonov**
CPP 49.1–49.10	Wed	15:00–17:45	C 230	**Soft Matter Physics: Emerging Topics, New Instruments and Methods**
CPP 50.1–50.8	Wed	15:00–17:15	C 243	**Charged Soft Matter, Polyelectrolytes and Ionic Liquids II**
CPP 51.1–51.7	Wed	15:00–17:00	C 264	**Hydrogels and Microgels**
CPP 52.1–52.6	Wed	15:00–16:30	PC 203	**Bioinspired Functional Materials, Biomaterials and Biopolymers (joint session CPP/BP)**
CPP 53.1–53.5	Wed	15:00–16:15	MA 144	**Solid-liquid interfaces: Reactions and electrochemisty III (joint session O/CPP)**
CPP 54.1–54.9	Wed	15:00–17:30	H 1028	**Microswimmers (joint session BP/CPP/DY)**
CPP 55.1–55.10	Wed	15:00–17:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials V (joint session O/MM/DS/TT/CPP)**
CPP 56.1–56.7	Wed	15:00–17:50	EMH 025	**Materials for Energy Storage II (joint session KFM/CPP)**
CPP 57.1–57.12	Wed	15:30–18:45	BH-N 243	**Active Matter (joint session DY/CPP/BP)**
CPP 58.1–58.7	Wed	16:00–18:15	H 0111	**Organic Thin Films, Organic-Inorganic Interfaces: Session I (joint session DS/CPP)**
CPP 59.1–59.5	Wed	16:45–18:00	MA 144	**Solid-liquid interfaces: Reactions and electrochemisty IV (joint session O/CPP)**
CPP 60.1–60.2	Wed	17:00–17:30	C 264	**Polymer and Molecular Dynamics I**
CPP 61.1–61.11	Thu	9:30–13:00	C 130	**Focus: Fundamental Physics of Perovskites II - organized by Lukas Schmidt-Mende and Vladimir Dyakonov**
CPP 62.1–62.13	Thu	9:30–13:00	C 243	**Charged Soft Matter, Polyelectrolytes and Ionic Liquids III**
CPP 63.1–63.13	Thu	9:30–13:00	C 264	**Polymer and Molecular Dynamics II**
CPP 64.1–64.12	Thu	9:30–12:45	PC 203	**Nanostructures, Nanostructuring and Nanosized Soft Matter II**
CPP 65.1–65.11	Thu	10:00–13:00	BH-N 333	**Granular Matter / Contact Dynamics (joint session DY/CPP)**
CPP 66.1–66.12	Thu	10:00–13:15	BH-N 243	**Microswimmers II (joint session DY/CPP/BP)**
CPP 67.1–67.9	Thu	10:30–12:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VI (joint session O/MM/DS/TT/CPP)**
CPP 68.1–68.5	Thu	11:45–13:00	C 230	**Crystallization, Nucleation and Self-Assembly I**

CPP 69.1–69.11	Thu	15:00–18:30	C 130	**Focus: Polymers in Multi-Compartment and Aqueous Solutions I - organized by Jens-Uwe Sommer and Debasish Mukheri**
CPP 70.1–70.11	Thu	15:00–18:15	C 230	**Crystallization, Nucleation and Self-Assembly II**
CPP 71.1–71.11	Thu	15:00–18:00	C 243	**Organic Electronics and Photovoltaics - OLEDs and Molecular Excitations**
CPP 72.1–72.10	Thu	15:00–18:00	C 264	**Hybrid and Perovskite Photovoltaics I**
CPP 73.1–73.6	Thu	15:00–16:30	PC 203	**Functional Polymer Hybrids and Composites**
CPP 74.1–74.10	Thu	15:00–17:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VII (joint session O/TT/MM/DS/CPP)**
CPP 75	Thu	18:45–19:45	C 130	**Annual General Meeting of the CPP Division (CPP Mitgliederversammlung)**
CPP 76.1–76.6	Fri	9:30–11:30	C 130	**Focus: Polymers in Multi-Compartment and Aqueous Solutions II - organized by Jens-Uwe Sommer and Debasish Mukheri**
CPP 77.1–77.12	Fri	9:30–13:00	C 243	**Organic Electronics and Photovoltaics - Transport and Doping**
CPP 78.1–78.12	Fri	9:30–12:45	C 264	**Hybrid and Perovskite Photovoltaics II**
CPP 79.1–79.8	Fri	9:30–11:30	PC 203	**Wetting, Microfluidics and Confined Liquids II**
CPP 80.1–80.6	Fri	9:30–11:00	H 0111	**Organic Thin Films, Organic-Inorganic Interfaces: Session II (joint session DS/CPP)**
CPP 81.1–81.10	Fri	9:30–12:00	H 1058	**Active Matter (joint session BP/CPP/DY)**
CPP 82.1–82.9	Fri	9:30–12:00	H 2013	**Membranes and Vesicles II (joint session BP/CPP)**
CPP 83.1–83.10	Fri	9:30–12:30	H 2032	**2D Materials (Symposium and Joint Session with HL and O): Session III (joint session DS/CPP/HL)**
CPP 84.1–84.10	Fri	10:00–12:45	BH-N 334	**Glasses and Glas transition (joint session DY/CPP)**
CPP 85.1–85.4	Fri	10:30–11:30	MA 144	**Molecular films: Photovoltaics, electronics and morphology (joint session O/CPP)**
CPP 86.1–86.9	Fri	10:30–12:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VIII (joint session O/TT/MM/DS/CPP)**

Annual General Meeting of the Chemical and Polymer Physics Division

Thursday 18:45–19:45 C 130

CPP 1: Focus: Molecularly Functionalized Low-Dimensional Systems I - organized by Antonio Setaro, Carola Meyer, Aravind Vijayaraghvan and Matteo Mannini

Low dimensional nanostructures like nanotubes, wires and 2D molecular layers allow for the investigation of physics in reduced dimensions. These low dimensional systems can act as template for the alignment of molecules, which can assume the role of additional building blocks. The resulting functionalized nanostructures can have tailored chemical, optical, magnetic, or electronic properties. Controlled functionalization therefore promotes new device applications such as the detection of spin states in magnetic molecules by electronic transport or the monitoring of molecular switching events using local optical probes. This interdisciplinary focus session aims to gather experts from different fields to promote synergy effects between synthesis, microscopy, spectroscopy, electronics and engineering. The low dimensional materials that are the basis for further functionalization include - carbon and inorganic nanotubes - semiconducting and metallic nanowires - graphene nanoribbons - 2D nanostructures and can be functionalized with molecules or nanoparticles with peculiar magnetic, optical or electronic properties promoting new physical properties and/or offers new opportunities for devices.

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

Topical Talk CPP 1.1 Mon 9:30 C 130

Diameter-dependent optical absorption and energy transfer from encapsulated dye molecules to single wall carbon nanotubes — •Sofie Cambré[1], Stein van Bezouw[1], Jochen Campo[1], Joeri Defillet[1], Wim Wenseleers[1], Dylan H. Arias[2], Rachelle Ihly[2], Andrew J. Ferguson[2], Justin C. Johnson[2], and Jeffrey L. Blackburn[2] — [1]Physics Department, University of Antwerp, Antwerp, Belgium — [2]Chemistry & Nanoscience Center, National Renewable Energy Laboratory, Golden Colorado, USA

The hollow core and well-defined diameters of single-walled carbon nanotubes (SWCNTs) allow for creation of unique one-dimensional hybrid structures by encapsulation of various molecules.[1] Here, we show that the optical properties of dye molecules encapsulated in SWCNTs can be strongly modulated by the SWCNT diameter, indicating very specific diameter-dependent stacking and interactions of the molecules. The filling is thoroughly characterized by optical absorption, resonant Raman, and two-dimensional infrared photoluminescence excitation (PLE) spectroscopy. Energy transfer probed by PLE spectroscopy shows the absorption spectrum of the dyes to be strongly diameter-dependent. The design of these functional hybrid systems, with tuneable dye absorption demonstrates potential for implementation in dedicated photo-conversion devices.

[1] S. Cambré, J. Campo et al., Nature Nanotechnol. 10, 248 (2015).

CPP 1.2 Mon 10:00 C 130

Encapsulation of molecules into carbon and boron nitride nanotubes - a comparison — •Katalin Kamarás[1], Áron Pekker[1], Dániel Datz[1], Hajnalka M. Tóháti[1], Kate E. Walker[2], Graham A. Rance[2], and Andrei N. Khlobystov[2] — [1]Wigner Research Centre for Physics, Budapest, Hungary — [2]University of Nottingham, Nottingham, United Kingdom

Encapsulation of small molecules into carbon nanotubes enables the study of special one-dimensional structures as well as chemical reactions in the cavities. We compare encapsulated structures using two kinds of nanotubes: carbon, with an extended π-electron system, and boron nitride, an analogue of carbon nanotubes with a predominantly ionic bonding. The different electronic structures give rise to different behavior in many aspects. Van der Waals interaction between the tube wall and the encapsulated molecule is much weaker in boron nitride, therefore the filling is easily reversible by solvent extraction. Boron nitride being transparent in most of the infrared and visible region, reactions within the tube can be followed by spectroscopy. On the other hand, the strong phonon-polariton mode and the local infrared-active defect modes can be detected by near-field spectroscopy, making it possible to map the defect structure with spatial resolution of the order of a few tens of nanometers. By thermal reactions, different kinds of double-walled nanotubes are produced, including "shielded nanocables" of carbon nanotubes inside boron nitride nanotubes.

CPP 1.3 Mon 10:15 C 130

Carbon nanotubes as templates for 1D nanostructures via a one-reactant-one-pot method — •Thomas Chamberlain — University of Leeds, Leeds, UK

Harnessing functional properties which emerge at the nanoscale is the key to developing superior materials for catalytic, electronic and biomedical applications. The internal cavity of single-walled carbon nanotubes provides an effective template for control of the exact positions and orientations of molecules and atoms and has been successfully applied to the construction of nanoscale architectures from a variety of metals, organic molecules, and inorganic compounds [1-3]. Low-dimensional inorganic materials, including transition metal chalcogenides, are of particular interest as their semiconducting properties can be precisely tuned by shaping their structures into nanoribbons. While the host-nanotube can control the dimensions of the inorganic structure, the stoichiometry is much more difficult to control.

An all-in-one molecular precursor that contains all necessary elements in correct proportion for the desired product, encapsulated in SWNTs and subsequently converted into the nanomaterial offers a highly effective solution to this challenge. This new strategy for nanoribbon synthesis and characterisation at the nanoscale can enable the formation of previously inaccessible quasi one-dimensional nanomaterials suitable for a variety of technological applications.

References: 1), T. Chamberlain et al., ACS Nano, 11(3), 2509-2520 (2017), 2), A. Botos et al., J. Am. Chem. Soc., 138(26), 8175-8183 (2016), 3), C. Stoppiello et al. Nanoscale, 9, 14385-14394, (2017).

CPP 1.4 Mon 10:30 C 130

Peapods with endofullerene single-molecule magnets — •Rasmus Westerström[1], Fabian Fritz[2,3], Christin Schleier[4], Stanislav M Avdoshenko[4], Alexey A Popov[4], and Carola Meyer[2,3] — [1]Synchrotron Radiation Research, Lund University, 22100 Lund, Sweden — [2]Department of Physics, University Osnabrück, 49076 Osnabrück, Germany — [3]Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [4]Leibniz Institute for Solid State and Materials Research (IFW), 01069 Dresden, Germany

Rare-earth-based endofullerene nanomagnets belong to the group of single-molecule magnets (SMMs), a class of molecules that exhibits an intrinsic magnetic bistability at low temperatures. Here we present a structural, chemical, and magnetic characterization of one-dimensional chains of endofullerene nanomagnets encapsulated in carbon nanotubes (CNTs), so-called peapods. It is demonstrated that unique peapod bundles can be located and studied by scanning transmission X-ray microscopy (STXM) and high-resolution transmission electron microscopy (HRTEM). By correlating HRTEM and STXM images, we show that structures down to 30 nm are resolved with chemical contrast and record nanoscale X-ray absorption spectra from endohedral lanthanide ions embedded in individual CNT bundles. Magnetic characterization of samples consisting of bundles of CNTs filled with $Dy_2ScN@C_{80}$ SMMs was performed using X-ray magnetic circular dichroism (XMCD), and the magnetic properties of these one-dimensional arrays will be discussed.

CPP 1.5 Mon 10:45 C 130

[Selective covalent functionalization of carbon nanotubes activated by light — •Georgy Gordeev[1], Thomas Rosenkranz[2], Stephanie Reich[1], and Ralph Krupke[2,3] — [1]Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institute of Materials Science, Technische Universitat Darmstadt, Darmstadt, Germany — [3]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

The diazonium reaction on nanotubes has recently attracted attention due to the ability of forming bright, fluorescent quantum defect states. The resonant light has been reported to accelerate and tune the reaction velocity. The latter is proportional to the energetic difference between transition energy and incident light. In our study, we demonstrate how a single chirality can be preferably functionalized by tuning optical excitation. We have performed the functionalization on a mixed chirality sample, resonantly exciting (9,7) tube. We monitored the reaction in situ via Raman spectroscopy. A dramatic difference between dark and illuminated areas in the functionalization degree was observed. The material outside the active spot did not demonstrate any changes from the pristine sample. The successful functionalization of the illuminated material was confirmed by resonant Raman scattering. The shift of transition energies and the number of sp3 defects was significantly higher in the resonantly excited nanotubes. The optically induced selectivity of the diazonium reaction paves a way of tuning and improving photonic devices based on nanotubes and can allow a large-scale single chirality enrichment of nanotubes.

15 min. break

Topical Talk CPP 1.6 Mon 11:15 C 130

Self-organization and energy transfer in non-covalent porphyrin - carbon nanotube supramolecular hybrids — Géraud Delport[2], Jean-Sébastien Lauret[2], Stéphane Campidelli[3], Fabien Vialla[1], and •Christophe Voisin[1] — [1]Laboratoire Pierre Aigrain, Ecole Normale Supérieure, Université Paris Diderot, Paris, France — [2]Laboratoire Aimé Cotton, Université Paris Saclay, Orsay, France — [3]LICSEN, CEA, Saclay, France

Functionalization of nanostructures with organic dyes brings the power and flexibility of organic chemistry to the nano-world and extends considerably the range of applications of nanomaterials. Nevertheless, covalent grafting of molecules may be detrimental to the intrinsic properties of the nano-object, whereas purely noncovalent approaches often yield assemblies of poor stability. We developed a micelle assisted supramolecular chemistry to create stable noncovalent complexes of porphyrin molecules attached to single-wall carbon nanotubes. We show that the stability of this assembly is partly due to porphyrin-porphyrin intra-layer interactions yielding a self-organized layer of porphyrin molecules with long-range ordering of the porphyrin orientation with respect to the nanotube axis. This arrangement results in original optical properties of the compound with polarization selective energy transfer. We discuss possible applications of this approach to the metrology of carbon nanotubes.

CPP 1.7 Mon 11:45 C 130

Surface magnetism of self-assembled metallofullerenes on metals — Denis Krylov[1], Chia-Hsiang Chen[1], Fupin Liu[1], Lukas Spree[1], Stanislav Avdoshenko[1], Sebastian Schimmel[1], Rasmus Westerström[2], Jan Dreiser[3], Christian Hess[1], and •Alexey Popov[1] — [1]Leibniz Institute for Solid State and Materials Research, Dresden. Germany — [2]Synchrotron Radiation Research Lund University, Sweden — [3]Swiss Light Source, Paul Scherrer Institut, Villigen PSI, Switzerland

Molecules with bistable magnetic ground state and slow relaxation of magnetization are known as single molecule magnets (SMMs). Information storage or spintronic applications envisaged for SMMs require contacting the molecules to conducting electrodes. Therefore, magnetic properties of SMMs on such surfaces should be well understood. However, whereas hundreds of transition metal and lanthanide based SMMs have been (and are being) reported, the studies of surface magnetism in monolayers of SMMs are very scarce, and hysteresis of magnetization on conducting substrates has been observed so far only for TbPc2, Fe4, and Dy2ScN@C80.

Endohedral metallofullerenes DyScN@C80 and Dy2ScN@C80 are robust SMMs combining structural stability with relatively high blocking temperature of magnetization, which allows their sublimation or chemical modification without decomposition of the magnetic core. In this work we use Scanning Tunneling Microscopy and X-ray magnetic circular dischroism to study structural and magnetic properties of submonolayers of metallofullerenes assembled on metallic substrates.

CPP 1.8 Mon 12:00 C 130

Spin-resolved photoemission measurements on a Fullerene monolayer adsorbed on Cu(111) — •Henning Sturmeit[1], Laura Kugler[1], Johannes Stöckl[2], Benito Arnoldi[2], Davide Bossini[1], Benjamin Stadtmüller[2], Martin Aeschlimann[2], Stefano Ponzoni[1], and Mirko Cinchetti[1] — [1]Experimentelle Physik VI, TU Dortmund, 44227 Dortmund, Germany — [2]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

Spin-resolved photoemission is a powerful method for the study of metal-organic interfaces. It allows to directly probe the effects of the interaction between the organic adsorbate and the metallic substrate on their electronic structure as well as its influence on the spin properties of the interface. In a recent work [1] it was reported that layered structures of C60 and metallic thin films show emerging ferromagnetic properties even with dia- or paramagnetic metals. Strong indications that the magnetic moment is localized in the metallic layer as well as at the interface were reported, although the physical origin of the ferromagnetic ordering is not yet fully understood. In this framework we performed spin-resolved photoemission measurements on an 4X4 - C60 monolayer absorbed on a Cu(111) surface. We found spin polarized photoemission features in the valence band of the system, although no clear signature of ferromagnetic ordering is detected.

[1] F. Al Ma'Mari, T. Moorsom, G. Teobaldi et al., Nature, 524 (7563), 69-73 (2015)

CPP 1.9 Mon 12:15 C 130

Magnetic behavior of Single Molecule Magnets thin films on low dimensional substrates — •Giulia Serrano[1], Irene Cimatti[1], Brunetto Cortigiani[1], Emilio Velez-Fort[2], Luigi Malavolti[3], Davide Betto[2], Nicholas B. Brookes[2], Abdelkarim Ouerghi[4], Edwige Otero[5], Matteo Mannini[1], and Roberta Sessoli[1] — [1]Department of Chemistry and INSTM RU, University of Florence, Via della Lastruccia 3, 50019, Sesto Fiorentino (FI), Italy. — [2]European Synchrotron Radiation Facility, 71, avenue des Martyrs CS 40220, 38043 Grenoble Cedex 9, France. — [3]Max-Planck Department for Structural Dynamics, Luruper Chaussee 149, 22761 Hamburg, Germany. — [4]Centre de Nanosciences et de Nanotechnologies, Université Paris-Sud, Université Paris-Saclay, C2N Marcoussis, 91460 Marcoussis, France. — [5]Synchrotron SOLEIL, L'Orme des Merisiers, Saint Aubin BP48 91192 Gif-sur-Yvette Cedex, France.

Single Molecule Magnets (SMMs) represent suitable building blocks for spintronic applications. Up to now, the intensive research to confine SMMs on solid substrates has shown promising results for Fe4 complexes SMMs on metal substrates. However, strong molecular interactions with the substrate may have detrimental effects on the SMMs magnetic properties, necessitating further exploration to be fully understood. Here we present the study of single-layers of the archetypal bis(phthalocyaninato) Terbium(III) complex (TbPc2) SMM on low-dimensional substrates as graphene and TiO2 nanoislands, demonstrating that the use of graphene results an effective strategy for preserving the magnetic bistability of SMMs.

CPP 1.10 Mon 12:30 C 130

Lanthanide-Functionalised Two Dimensional Transition Metal Dichalcogenides — •David Lewis — School of Materials, University of Manchester

Nanostructures provide a unique platform on which to assemble molecular layers.[1] Functionalisation of transition metal dichalcogenides (TMCDs) in particular, provides a facile route by which to produce new advanced composite nanomaterials that have advanced optoelectronic properties.[2]

Assembly of molecular lanthanide (III) complexes onto two-dimensional TMDCs provides an attractive opportunity by which to extend the latters advanced materials properties. For example, we have recently shown that 2D molybdenum disulfide nanosheets can be functionalised with both Eu3+ and Gd3+ complexes simultaneously.[3] The resulting nanomaterials display long photoluminescence emission lifetimes of 0.8 ms from the Eu3+ emission in the red region of the electromagnetic spectrum (570 to 720 nm), derived from the 5D0 to 7Fj electronic f-f transitions, whilst having strong paramagnetic response in EPR spectra, and thus could be used as a bimodal optical probe / magnetic resonance imaging contrast agent. The approach could be extended by exploring the whole range of lanthanide elements available for assembly on 2D surfaces. This talk will explore the feasibility of these exciting possibilities.

References [1] (a) Lewis et al, Chem Commun, 2006, 1433, (b) Lewis et al Coord. Chem. Rev. 2014, 273, 213. [2] Knirsch et al ACS Nano 2015, 9, 6018. [3] McAdams et al, Adv Func. Mater. 2017, 1703646.

CPP 1.11 Mon 12:45 C 130

Magnetic subunits within a single molecule-surface hybrid —

•Rico Friedrich[1,4], Volkmar Hess[2,3], Vasile Caciuc[1], Frank Matthes[2], Daniel E. Bürgler[2], Nicolae Atodiresei[1], Claus M. Schneider[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [3]Institut für Anorganische Chemie, RWTH Aachen University, D-52074 Aachen, Germany — [4]Present address: Center for Materials Genomics, Duke University, Durham, NC 27708, USA

Single molecule-surface hybrid systems are a promising platform for molecular spintronics due to their adjustable magnetic properties [1, 2]. In this contribution we demonstrate the creation of multiple intramolecular subunits within a single molecule-surface hybrid system employing *ab initio* density functional theory and spin-polarized scanning tunneling microscopy [3].

Upon deposition of a polycyclic aromatic molecule onto a ferromagnetic surface an asymmetric (chiral) adsorption geometry is obtained. This gives rise to the formation of different structural, electronic and magnetic properties of each aromatic ring hybridizing with the surface. Finally, this leads to the creation of magnetic subunits which are distinguished from one another by their exchange coupling strength [3].

[1] N. Atodiresei *et al.*, Phys. Rev. Lett. **105**, 066601 (2010).
[2] R. Friedrich *et al.*, Phys. Rev. B **91**, 115432 (2015).
[3] V. Heß *et al.*, New J. Phys. **19**, 053016 (2017).

CPP 2: Electrical, Dielectrical and Optical Properties of Thin Films I

Time: Monday 9:30–11:00 Location: C 230

CPP 2.1 Mon 9:30 C 230

Singlet fission in pentacene blends with tunable charge-transfer interactions — •Katharina Broch[1], Johannes Dieterle[1], Federico Branchi[2], Nicholas Hestand[3], Yoann Olivier[4], Hiroyuki Tamura[5], Chad Cruz[6], Valerie Nichols[6], Alexander Hinderhofer[1], David Beljonne[4], Francis Spano[3], Giulio Cerullo[2], Christopher Bardeen[6], and Frank Schreiber[1] — [1]Universität Tübingen, Tübingen, Germany — [2]Politecnico di Milano, Milano, Italy — [3]Temple University, Philadelphia, Pennsylvania, USA — [4]University of Mons, Mons, Belgium — [5]Tokyo University, Tokyo, Japan — [6]University of California at Riverside, Riverside, USA

Singlet fission (SF), which transforms an excited singlet state into two triplet states, is receiving increasing attention due to its potential to boost organic solar cell efficiencies [1]. While the key role of intermolecular charge transfer in SF has been demonstrated [2], the impact of reduced intermolecular interactions on SF time scales is not yet fully understood. To gain deeper insight, a continuous modification of the interaction strength between the two extremes of isolated chromophores and single crystals would be valuable, but remains challenging. We demonstrate the possibility to modify charge transfer interactions of pentacene, a prototypical SF material [3], in blends with weakly interacting spacer molecules and discuss the impact on SF time constants in these mixed films.

[1] M. Smith and J. Michl, Chem. Rev. 110 (2010), [2] B. Basel et al., Nat. Comm. 8 (2017), [3] M. Wilson et al., JACS 133 (2010).

CPP 2.2 Mon 9:45 C 230

Investigation of Charge Carrier and Electric Field Distribution in OLEDs by Means of Photoluminescent Molecular Probes — •Thomas Ferschke[1] and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

Recently, it has been shown that current densities can be determined on nanometer length scales by means of photoluminescence (PL) studies on single guest dye molecules.[1] Here we transfer this concept to common Alq_3/α-NPD OLEDs by utilizing Tetraphenyldibenzoperiflanthene (DBP) entities as molecular probes. DBP is intentionally embedded as dopant (0.1 v-%) at defined depth within the Alq_3 emissive layer. Upon charge injection a reduction in dopant PL is observed which can be attributed to non-radiative electron - exciton interaction. The macroscopic current density scales related to the PL quenching with the distance from the injecting electrode in qualitative agreement with a SCLC model. The validity of this model and thus, variations in vertical charge carrier distribution are studied as a function of current density. Even at reverse bias condition PL quenching of DBP guest molecules in proximity of 5 nm to the Alq_3/α-NPD interface is observed. This can be attributed to strong localized electric fields at the interface caused by interfacial charges of Alq_3.[2] In addition to quenching measurements a comparative study on the integral interface charging is performed by means of impedance spectroscopy.

[1] Nothaft *et al.*, *ChemPhysChem*, **2011**, 12, 2590–2595
[2] Noguchi *et al.*, *J. Appl. Phys.*, **2012**, 111(11):114508

CPP 2.3 Mon 10:00 C 230

Advanced synthesis of transparent and conductive poly(3,4-ethylenedioxy thiophene) films via vapor-based routes — •Florian Meierhofer[1,2], Laurie Neumann[1,3], Wolfgang Kowalsky[1,3], Hans-Hermann Johannes[1,3], and Tobias Voss[1,2] — [1]Laboratory for Emerging Nanometrology (LENA), TU Braunschweig, Germany — [2]Institute of Semiconductor Technology (IHT), TU Braunschweig, Germany — [3]Institute of High-Frequency Technology (IHF), TU Braunschweig, Germany

Conducting polymers (CP) combine the electrical properties of semiconductors and metals with mechanical flexibility and stretch of insulating polymers, and therefore offer a huge potential for light emitting diodes (LEDs) and photovoltaics (PV). During the past two decades, PEDOT:PSS has become one of the most attractive CPs and is often applied in spin-coated 2D-layers. The coating of more complicated 3D-surfaces, e.g. nanowires/-trenches, however, typically results in an incomplete surface coverage. This issue can be overcome by applying the polymerization directly from the vapor phase. In this work, we use vapor-phase polymerization (VPP) and oxidative chemical vapor deposition (oCVD) for the fabrication of layers of PEDOT and other thiophene derivatives. Aiming for high transparency and electrical conductivity, we systematically screen oxidizing agents and polymerization temperatures. First results for the vapor-synthesized PEDOT demonstrate a transparency of about 90% and 5 S/cm electrical conductivity, which is even superior to PEDOT:PSS as the commercial benchmark.

CPP 2.4 Mon 10:15 C 230

Investigation of the n-type polymer P(NDI2OD-T2) for thermoelectric applications — •Regina Michaela Kluge, Nitin Saxena, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Thermoelectric generators pose a promising approach in renewable energies as they are able to convert waste heat into electricity. In order to build high efficiency devices, suitable thermoelectric materials are needed. Among them, conjugated polymers possess the encouraging ability of easy and various types of scalable solvent processes like roll-to-roll printing. Although they are still less efficient than their inorganic counterparts, their easy synthesis, flexibility and eco-friendliness make them a valuable alternative. However, in order to build a thermoelectric device, both n- and p-type materials are needed. Whereas p-type polymers are frequently studied, n-type polymers have often been neglected in the past which may originate from their sensitivity towards oxygen and moisture. We investigate the air-stable, high-mobility n-type polymer P(NDI2OD-T2) in terms of its optical properties such as its absorbance. Moreover, thermoelectric properties such as the Seebeck coefficient and the electrical conductivity are probed, which allows to determine the power factors of these films.

CPP 2.5 Mon 10:30 C 230

Investigating optical excitations in push-pull molecular J-aggregates by TDDFT first-principles simulations — •Michele Guerrini[1,2], Arrigo Calzolari[2], and Stefano Corni[2,3] — [1]Dept. of Physics, Information and Mathematics , University of Modena and Reggio Emilia, Italy — [2]CNR Nano Modena, Italy — [3]Dept. of Chemical Sciences, University of Padova, Italy

J-aggregates are a class of molecular crystals which show interesting optical properties such as an intense and narrow red-shifted absorption peak (aka J-band) with respect to the monomer units they are composed of. In this work we investigated the electronical optical properties of a J-aggregate molecular crystal made of ordered arrangements of organic push-pull chromophores. By using a TDDFT first-principles approach, we assessed the role of molecular packings in the formation of the enhanced and red-shifted J-band and the major effects of confinement in the optical absorption when moving from bulk to low-dimensional crystal structures. In particular, we simulated the optical absorption of different configurations (i.e. monomer, dimers, extended polymer chain and monolayer sheet) obtained from the bulk crystal. By analyzing the induced charge density associated to the J-band, we concluded that this characteristic peak is mostly associated to a longitudinal excitation that is delocalized along linear chains within the bulk crystal and its red-shift is explained in terms of couplings between transition densities along these chains, as well as changes in single particle excitations, that lowers the total excitation energy.

CPP 2.6 Mon 10:45 C 230

Study on conductive silver nanowire networks in 3D printed polymers — •Lewis Akinsinde[1], Tomke Glier[1], Ferdinand Otto[1], Calvin J. Brett[2,3], Milena Lippmann[3], Stephan V. Roth[3,4], and Michael A. Rübhausen[1] — [1]Institut für Nanostruktur und Festkörperphysik, Universität Hamburg — [2]Department of Fluid Physics, Royal Institute of Technology (KTH), Stockholm, Sweden — [3]Photon Science, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [4]Royal Institute of Technology (KTH), Stockholm, Sweden

Nowadays, increasing attention has been devoted to transparent conductive films because of their various applications in Solar cells and OLEDs. 3D printing is an alternative promising fabrication process. The embedding of silver nanowires in a UV sensitive polymer matrix enables 3D printable conductive objects. Hence silver nanowires were synthesized via the polyol method resulting in an average diameter of approximately 130 nm and a length up to 100 μm. With optimization through dry etching sheet electrical resistance could be reduced to ca. 1.5 Ω/square. This is highly competitive with existing candidates such as indium tin oxide (ITO). As a next step layer systems consisting of UV cured 1,6-Hexanediol diacrylate (HDDA) and silver nanowires were prepared. The structure and morphology of the silver nanowire incorporated thin films were investigated by scanning electron microscopy (SEM), atomic force microscopy (AFM), conductivity measurements and spectroscopic measurements. Inner film morphology was studied using grazing incidence small-angle X-ray scattering (GISAXS)

CPP 3: Organic Electronics and Photovoltaics - Layer Morphology and Molecular Aggregation

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

Invited Talk CPP 3.1 Mon 9:30 C 243

Time-resolved in-situ x-ray scattering to resolve structure formation in thin film processing — •Eva M. Herzig — Universität Bayreuth, Physikalisches Institut, Herzig Group - Dynamik und Strukturbildung, 95440 Bayreuth, Germany

The nanomorphology of thin films determines a wide range of physical properties and therefore the performance of functional thin films. Typical examples are found in organic electronics as in organic or hybrid photovoltaics. Understanding the self-assembly processes that occur during the drying of the photoactive film, will allow us to make progress in controlled nanomorphology tuning. We have developed tools to investigate thin film formation processes using synchrotron radiation to resolve structural developments with time [1]. We can control various processing parameters to systematically investigate the influence of these parameters on the final thin film morphology. This allows us, for example, to resolve the temporal evolution of polymer crystallization processes [2]. We complement the structural analysis with time-resolved spectroscopy measurements to gain further understanding on the structure formation processes. In this talk, the influence of the deposition environment is discussed and its role for controlling the thin film morphology and the resulting material properties. - - - [1] S. Pröller et al. "Note: Setup for chemical atmospheric control during in situ grazing incidence X-ray scattering of printed thin films" Rev. Sci. Instrum. 2017, 88(6): 066101. [2] S. Pröller et al. "Following the Morphology Formation In Situ in Printed Active Layers for Organic Solar Cells" Adv. Energy Mater. 2016, 6(1): 1501580.

CPP 3.2 Mon 10:00 C 243

The impact of morphology and polymer-fullerene miscibility on device stability of organic solar cells — •Andrej Classen, Chaohong Zhang, Yakun He, Heumueller Thomas, Ning Li, Jose Dario Perea, Stefan Langner, and Christoph Brabec — FAU Erlangen-Nürnberg, Germany, Erlangen

As organic PV efficiencies regularly exceed 10%, the science of stabilization and lifetime gains importance. Several degradation phenomena in organic solar cells are related to an increase in trap density, and have been studied with respect to their impact on open-circuit voltage and fill factor. The short circuit current may be affected by fullerene dimerization which shows a clear dependence on active layer morphology and can be avoided by using different fullerene derivatives. Interestingly, in several novel high performing polymers, such as PTB7 and PCE11, intrinsic morphological instabilities have been observed. Utilizing different fullerene derivatives, we find that increased solubility of the fullerene within the polymer matrix allows superior device stability, but can reduce the initial device performance. Thus a fine balance between stability and device performance has to be found by tuning the donor-acceptor ratio in those systems. To separate effects from several different degradation mechanisms that usually occur at the same time, we perform tests under controlled environmental conditions to avoid photo-oxidation and distinguish between thermal and light induced degradation by applying a series of temperature steps in the dark.

CPP 3.3 Mon 10:15 C 243

investigating the degradation of PffBT4T-2OD: PCBM solar cells by in-operando GISAXS/ GIWAXS measurements — •Dan Yang[1], Franziska C. Löhrer[1], Volker Körstgens[1], Armin Schreiber[1], Sigrid Bernstorff[2], Jillian Buriak[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Elettra Sincrotrone Trieste, Basovizza, 34149 Trieste, Italy — [3]University of Alberta, Department of Chemistry, Edmonton, Canada

Polymer bulk heterojunction solar cells are showing great potential as a cost-effective alternative to conventional solar cells in near future due to their easily scalable and solution-based manufacturing. The power conversion efficiencies (PCE) of lab-scale devices have already exceeded 13%. Aside from optimizing the initial PCE of solar cells, their long-term stability must be considered as a key role in the organic solar cell (OSCs) development. The degradation of OSCs mainly focuses on the role of oxygen, water and intrinsic degradation of constituent materials. To investigate the degradation behaviour of the donor material in organic solar cells, PffBT4T-2OD: PC71BM solar cells are probed with in-operando GISAXS and GIWAXS measurements. From the combination of the morphology changes with the J-V performance, the degradation mechanisms can be well understood. This should be very important for optimizing the individual materials to improve the stability of organic solar cells.

CPP 3.4 Mon 10:30 C 243

Influence of solvent additive 1,8-octanedithiol on P3HT:PCBM solar cells — Weijia Wang[1], Lin Song[1], David Magerl[1], Daniel Mosegui Gonzales[1], Volker Körstgens[1], Martine Philipp[1], Jean-Francois Moulin[2], and •Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]HZG at MLZ, 85747 Garching

Organic solar cells based on poly(3-hexylthiophen-2,5-diyl):phenyl-C60-butyric acid methyl ester (P3HT:PCBM) have developed into a well-controlled model system for studying fundamental questions, although device efficiencies of other blends using low band gap polymers demonstrated significantly higher device efficiencies. We investigate the influence of solvent additive 1,8-octanedithiol (ODT) on polymer crystallinity, surface and inner morphology, and quantitative molecular miscibility of P3HT and PCBM as function of the ODT volume concentration. The crystallinity is probed with absorption spectroscopy and grazing incidence wide angle X-ray scattering. The morphology and miscibility are characterized via AFM and time-of-flight grazing incidence small angle neutron scattering. ODT processing proves to be beneficial for promoting P3HT crystallinity and optimizing the inner morphology in terms of substructures and molecular miscibility, consequently leading to a better photovoltaic performance.

CPP 3.5 Mon 10:45 C 243

Effect of Side Chain Modification on Crystallization and Crystal Orientation in Thin Films of Poly(3-(6-bromohexyl)-thiophene) — •Oleksandr Dolynchuk[1], Philip Schmode[2], Paul M. Reichstein[2], Matthias Fischer[1], Mukundan Thelakkat[2], and Thomas Thurn-Albrecht[1] — [1]Experimental Polymer Physics, Institute of Physics, Martin Luther University Halle-Wittenberg, Germany — [2]Applied Functional Polymers, Macromolecular Chemistry I, University of Bayreuth, Germany

Semicrystalline conjugated polymers are of great interest as organic materials for various electronic devices due to a remarkable combination of semiconducting, thermal and mechanical properties, which strongly depend on morphology and orientation of polymer crystals. This work aims a comparative study of crystallization of poly(3-(6-bromohexyl)-thiophene) (P3BrHT) and poly(3-hexylthiophene) (P3HT) in bulk and in thin films. Differential scanning calorimetry evidenced a significant decrease of crystallization and melting temperatures and melting enthalpy of P3BrHT as compared to P3HT. Temperature dependent wide-angle XRD revealed a distortion of crystal lattice in bulk P3BrHT and allowed estimating crystallinity in this material that amounted to about 43%. The crystal orientation in ultrathin films of both polymers spin coated on SiO_2/Si and graphene was explored using grazing incidence XRD. The results indicated stronger face-on crystal orientation with π-π stacking normal to both substrates in as-spun P3BrHT than P3HT, whereas melt-crystallized P3BrHT on graphene has only face-on oriented crystals.

15 min. break

CPP 3.6 Mon 11:15 C 243

Studying lamellar-like morphologies of conjugated polymers through a new symmetry-inspired model — •Cristina Greco, Kurt Kremer, and Kostas Daoulas — Max Planck Institute for Polymer Research, Mainz, Germany

In conjugated polymers, charge transport properties are known to be strongly affected by morphology. An interesting recent observation is that, to achieve high mobilities, perfect lamellar order is not necessary [1]. Here we present a simple model that enables the study of morphologies with partial lamellar order, at device-relevant length scales. Nonbonded interactions responsible for coplanarity in chain orientation and for stacking are described by anisotropic soft potentials constructed on the basis of symmetry considerations. Using polyalkylthiophenes as a test system, we perform Monte Carlo simulations of chains of various lengths. Lamellar-like morphologies are obtained, either as mono- or polydomains. The type of lamellar order is identified by computing 2D scattering patterns, which can be compared with experimental GIWAXS data. From this analysis, we conclude that our morphologies correspond to a smectic mesophase, which was also reported in experiments [2]. We analyze the organization of chains inside the lamellae and identify in a simple way connectivity pathways between the lamellae. In perspective, atomistic detail can be reintroduced via backmapping, allowing for prediction of charge transport [3]. [1] R. Noriega et al. Nat. Mater. 2013, 12, 1038. [2] Z. Wu et al. Macromolecules 2010, 43, 4646. [3] P. Gemünden et al. Macromol. Rapid Commun. 2015, 36, 1047.

CPP 3.7 Mon 11:30 C 243

Orientation and Order Bottle Brush Copolymers — •Arthur Markus Anton[1], Christian David Heinrich[2], Mukundan Thelakkat[2], and Friedrich Kremer[1] — [1]Peter Debye Institut for Soft Matter Physics, Leipzig University — [2]Macromolecular Chemistry I, University of Bayreuth

Compared to linear polymers bottle brush copolymers provide advantages, such as higher chain mobility or increased persistence length. Concerning this, a protocol on the preparation of brush copolymers containing electronically active poly(3-hexylthiophene) (P3HT) segments in their side chains has recently been published [1]. With rising side chains length highly crystalline materials are obtained; lamellar crystals have been observed *for the first time* in the case of brush copolymers. Moreover, the charge carrier mobility in brushes is comparable to linear P3HT, whereas the brushes' excellent thermal stability gives rise to further applications [1]. To analyze the molecular organization in the P3HT bottle brush films infrared transition moment orientational analysis (IR-TMOA) is employed [2,3]. The spectral absorption is recorded depending on the polarization *and in addition* on the inclination of the sample film relative to the incident light. This enables to determine the spatial orientation and order of particular molecule segments. While linear P3HT exhibits a distinct face on orientation, no macroscopic order is evident in the brush copolymer.

[1] C. D. Heinrich and M. Thelakkat, *J. Chem. Phys. C* **4** (2016) 5370
[2] A. M. Anton, F. Kremer et al., *J. Am. Chem. Soc.* **137** (2015) 6034
[3] A. M. Anton, F. Kremer et al., *Macromolecules* **49** (2016) 1798

CPP 3.8 Mon 11:45 C 243

Investigating molecules response toward laser illumination during laser directed self-assembly (LDSA) — •Andika Asyuda[1], Linus Pithan[1,2], Anton Zykov[1], Andreas Opitz[1], and Stefan Kowarik[1,3] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Berlin — [2]European Synchrotron Radiation Facility, Experiments Division ID03, Grenoble — [3]Bundesanstalt für Materialforschung und Prüfung, 8.6 Fibre Optic Sensors, Berlin

A growth of tetracene thin film is among intensively studied vapor-deposited molecular film. While tetracene is usually grown as randomly oriented polycrystalline film, Pithan et al [1] demonstrated a way to use laser illumination during thin film growth for aligning the growing crystallites in the film. The key of this approach is choosing a laser wavelength matching 1 of its 2 Davydov components.

An aligned crystalline film is indeed desirable for device realization, such as transistor, due to anisotropic carrier transport in organic semiconductors. However, there is no investigation yet of structural properties of photoaligned film, such as roughness, island surface area, and island density. In this contribution, various growth parameters of a photoaligned tetracene film are discussed, particularly for their influences to film morphology and anisotropy. Recent AFM data consistently show an increase in grain size due to photoalignment, regardless of substrate temperature and molecular flux during the growth.

[1] L. Pithan, et al, Adv. Mater. 2017, 29, 1604382

CPP 3.9 Mon 12:00 C 243

Impact of the excitation spot adjustment in angular resolved photoluminescence experiments — •Christian Hänisch, Simone Lenk, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, TU Dresden, Germany

One of the main pathways of optimizing the performance of organic light-emitting diodes (OLED) is the reduction of optical loss modes by aligning the transition dipole moments (TDM) of the light-emitting molecules parallel to the substrate interface.

Angular resolved photoluminescence spectroscopy is the most prominent experimental technique to determine the anisotropy factor as a measure of the average TDM orientation. Despite the widespread application of this method, a quantitative discussion of the impact of specific setup configurations is - to the best of our knowledge - missing so far. Especially, the accurate positioning and size of the optical excitation spot is very important as well as its distance to the detector.

With help of a numerically solved ray optics model, we show that already small displacements of the excitation spot can lead to remarkable changes in the measured emission spectra. For non-ideal setup configurations, the accuracy of experimental data fits can be drastically improved using the developed corrections.

Hence, this work enables not only to numerically treat unavoidable experimental non-idealities such as displacements caused by the substrate thickness but also helps to quantify and state measurement deviations of the anisotropy factor.

CPP 3.10 Mon 12:15 C 243

Control of molecular orientation on a single substrate by changing growth parameters leads to switching of thin-film optical properties — •Giuliano Duva[1], Linus Pithan[2], Alexander Gerlach[1], Alexander Janik[1], Alexander Hinderhofer[1], and Frank Schreiber[1] — [1]Eberhardt Karls Universität Tübingen, Tübingen, Germany — [2]European Synchrotron Research Facility (ESRF), Grenoble, France

The Optical response of many organic semiconductors (OSC) can exhibit anisotropy depending on the average orientation of the molecular components [1]. Diindenoperylene (DIP) is an OSC whose HOMO-LUMO transition dipole moment is parallel to the long molecular axis. Organic Molecular Beam Deposition (OMBD) allows a high degree of control over the thin film structure. Using OMBD, uniaxially ordered

DIP films in a standing-up configuration at room temperature are obtained exhibiting a strong optical anisotropy, with the out-of-plane component of the dielectric function being roughly ten times higher than the in-plane component in the visible spectrum [2]. Here we present a method to change the molecular orientation without modifying the substrate or reducing crystal quality. Growth via OMBD followed by annealing allows to obtain ordered, atmosphere-stable films of mostly lying-down DIP exhibiting inverted optical properties compared to films of standing-up DIP. We also discuss a possible mechanism to explain this effect.

[1] A. Hinderhofer et al. Chem. Phys. Chem. 13 (2012).
[2] U. Heinemeyer et al. Phys. Rev. B 78 (2008).

CPP 3.11 Mon 12:30 C 243

Elucidating Aggregation Pathways And Structural properties Of Chromophores With The Help Of MD-Simulations — •Axel Bourdick[1], Markus Reichenberger[2], Anna Köhler[2], and Stephan Gekle[1] — [1]Biofluid Simulation and Modeling, University of Bayreuth, 95440 Bayreuth (Germany) — [2]Experimental Physics II, University of Bayreuth, 95440 Bayreuth (Germany)

We investigate the aggregation behaviour of the donor-acceptor molecules pDTS(FBTTh2)2 (”T1”) and p-SIDT(FBTTh2)2 (”H1”) in MTHF solutions. Using optical spectroscopy, we find that T1 forms aggregates in solution while H1 aggregates only when processed as a thin film, but not in solution. Free energy molecular dynamics (MD) simulations based on force-fields derived from quantum-mechanical density functional theory fully reproduce this difference. Interestingly, our simulations reveal that this difference is not due to the lengthy carbon side chains. Instead, it can be traced back to the different molecular symmetry which allows T1 to form an aggregated state in which the central donor units are spatially well separated while a similar configuration is sterically impossible for H1. As a consequence, any aggregation of H1 necessarily involves aggregation of the central donors which requires, as a first step, stripping the central donor of its protective MTHF solvation shell. This unfavorable process leads to a significant kinetic hindrance for aggregation and explain the strongly differing aggregation behavior of T1/H1 in MTHF despite their otherwise similar structure.

CPP 3.12 Mon 12:45 C 243

H- an J-type electronic coupling in single conjugated polymer aggregates — •Theresa Eder[1], Thomas Stangl[1], Max Gmelch[1], Klaas Remmerssen[2], Dirk Laux[2], Sigurd Höger[2], Jan Vogelsang[1], and John Lupton[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg — [2]Kekulé-Institut für organische Chemie und Biochemie, Universität Bonn

Single-molecule spectroscopy (SMS) has proved to be a useful tool to further understand light and charge generation in organic semiconductors. However, it is not sufficient to unravel the various coupling processes between single polymer chains which take place in the organic layer of devices like an organic light emitting diode or solar cell. To bridge the gap between those thick layers and single molecules we grow single aggregates which consist of several single polymer chains. Depending on their morphology those aggregates can show distinct types of coupling which can be generally explained using the concept of H- and J-type coupling. Here we show not only that the type of coupling can be chosen by using modified polymers, but we can also switch reversibly between H- and J-type coupling of one and the same single aggregate by exposing it to solvent vapour. To distinguish between the different types of aggregates we examine them using SMS and extract their characteristic photophysical properties. This experiment contributes to a further understanding of electronic interactions between polymer chains in an aggregate and highlights the simultaneous existence of H- and J-type coupling in well-ordered aggregates [1].
[1] Eder et al., Nature Comm. 8, 1641 (2017)

CPP 4: Complex Fluids and Colloids I (joint session CPP/DY)

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

CPP 4.1 Mon 9:30 C 264

Brownian motion of a microbead coated with a temperature-responsive polymer brush layer — •David van Duinen, Dominik Pilat, Hans-Jürgen Butt, and Rüdiger Berger — Max Planck Institute for Polymer Research, Mainz, Deutschland

We report on a simple method that allows investigating the mechanical contact between a planar surface and a microbead that is covered with a thin stimuli-responsive polymer brush. The brush consists of linear poly(N-isopropylacrylamide) (PNIPAM), which has a lower critical solution temperature (LCST). Below the LCST, the brush is hydrated and extended. In contrast, above the LCST the polymer collapses; this system can be described using a spring model, which is stiffer in the collapsed state than in the hydrated state. Similarly, we have investigated the effect of cononsolvency on the mechanical contact.

This method allows the following and checking of the characteristics of thin polymer films upon exposure to stimuli. The method is simple, and provides information that is otherwise hard to obtain.

CPP 4.2 Mon 9:45 C 264

Polymer mediated interactions between colloids immersed in a polymer blend — •Alexander Chervanyov — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster

We analytically study the polymer mediated (PM) interactions between colloids immersed in a polymer blend. By making use of standard methods of the liquid state theory we have found out a novel mechanism of the PM interactions caused by non-uniformities in the local composition of the polymer blend induced by the colloids. The relative significance of the contributions to the PM interaction potential due to the finite compressibility of the polymer blend and its compositional non-uniformity is found to drastically depend on the polymer-to-colloid size ratio. In the protein limit of relatively small colloids, the mechanism due to the compositional non-uniformity, specific to polymer blends, is shown to play a dominant role in the PM interactions.

CPP 4.3 Mon 10:00 C 264

Spontaneous symmetry breaking of charge-regulated surfaces — •Arghya Majee[1], Markus Bier[1], and Rudolf Podgornik[2] — [1]MPI for Intelligent Systems, Stuttgart & University of Stuttgart, Germany — [2]J. Stefan Institute, Ljubljana & University of Ljubljana, Slovenia

The interaction between two chemically identical charge-regulated surfaces is studied using the classical density functional theory. In contrast to common expectations and assumptions, under certain realistic conditions we find a spontaneous emergence of disparate charge densities on the two surfaces [1]. The surface charge densities can differ not only in their magnitude, but quite unexpectedly, even in their sign, implying that the electrostatic interaction between the two chemically identical surfaces can be attractive instead of repulsive. Moreover, an initial symmetry with equal charge densities on both surfaces can also be broken spontaneously upon decreasing the separation between the two surfaces. These findings are fundamental for the understanding of the forces between colloidal objects and, in particular, they are bound to strongly influence the present picture of protein interaction.

Reference:
[1] A. Majee, M. Bier, and R. Podgornik, arXiv: 1709.05005 (2017).

CPP 4.4 Mon 10:15 C 264

PFA-PEG particles: A colloidal model system for the investigation of phase diagrams of PEGylated drug carrier systems — •Marcel Werner[1,2], Judith Ruland[2], Nils von Seggern[1], Moritz Tappe[1], Melanie Wernet[2], Gabriela Schmidt[2], and Eckhard Bartsch[1,2] — [1]Department of Macromolecular Chemistry, University of Freiburg, Freiburg im Breisgau, Germany — [2]Department of Physical Chemistry, University of Freiburg, Freiburg im Breisgau, Germany

Pegylated particles like proteins, peptides and lipid- or polymer-based nanoparticles are known as potential drug delivery systems (DDS) or as nano drug carriers (NDC) [1]. Current research deals with e.g. completely new systems [2], shape effects [3] or the influence of the PEG density on the biocompatibility [4]. However, the phase behaviour of the DDS is not really covered. In an attempt to close this gap we synthesised a new model system, consisting of a highly fluorinated core and a sterically stabilizing PEG-shell [5]. With these particles and different light scattering techniques as well as other complementary techniques such as microscopy and rheology, we gained first insights into the phase behaviour of PEGylated particles. Our findings can lead to higher concentrated carrier systems without unwanted inter particle interference and new formylations e.g. gels or cremes.

[1] T. M. Allen et al., Science, 2004, 303, 1818. [2] E. Ruiz-Hernandez et al., Polym. Chem., 2014, 5, 1674. [3] Y. Li et al., Nanoscale, 2015, 40, 16631. [4] J. L. Perry et al., Nano Lett., 2012, 12, 5304. [5] D. Burger et al., Colloids Surf. A: Physico. Eng. Aspects, 2014, 442, 123.

CPP 4.5 Mon 10:30 C 264

Interactions in Protein Solutions in the Vicinity of the Gas-Liquid Binodal — •Jan Hansen[1], Florian Platten[1], Jannik Nedergaard Pedersen[2], Jan Skov Pedersen[2], and Stefan U. Egelhaaf[1] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Department of Chemistry & iNANO, Aarhus University, Denmark

Intermolecular interactions in protein solution depend on a delicate balance of electrostatic, van der Waals and hydrophobic interactions, hydration and other specific contributions. Under certain conditions, short-ranged attractions dominate. Then, proteins can be described as adhesive hard spheres, i.e. their equilibrium phase diagram contains a solubility line below which the metastable gas-liquid binodal is submerged. Here, we examine in how far effective interaction models from colloid science can help to rationalize the phase behavior and interactions of protein solutions in the vicinity of the gas-liquid binodal. For different solution compositions, binodals have been determined by cloud-point measurements, yielding estimates of the critical temperature T_c. The effective structure factor of protein solutions has been determined for various protein concentrations and temperatures by small-angle X-ray scattering. The data is well described by a one-parameter fit based on Baxter's model, from which the second virial coefficient B_2 is inferred. If plotted as a function of temperature normalized by T_c, the values of B_2 follow a universal behaviour for various solution conditions, as suggested by the extended law of corresponding states.

CPP 4.6 Mon 10:45 C 264

Behavior under shear of solutions of bovine serum albumin and trivalent cations — •Stefano Da Vela[1], Miriam Siebenbürger[2], Alessio Zaccone[3], Fajun Zhang[1], Matthias Ballauff[2,4], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, University of Tübingen, Tübingen, Germany — [2]Helmholtz Zentrum für Materialien und Energie, Berlin, Germany — [3]Dept. of Chemical Engineering and Biotechnology, University of Cambridge, Cambridge, UK — [4]Department of Physics, Humboldt-University, Berlin, Germany

Trivalent cations such as Y(III) and La(III) have been shown to induce a rich phase behavior in aqueous solutions of acidic proteins. Thanks to the specific association of the cations with the negatively charged groups on the protein surface, these systems feature directional, patchy interactions. Here we show how shear stress can trigger aggregation in solutions of the acidic protein bovine serum albumin (BSA) in the presence of La(III). The trivalent cation renders the system unstable at high shear rates and the solutions become turbid. Simultaneously a low wavevector upturn develops in small-angle neutron scattering profiles. We discuss the findings in relations to the available theoretical models. As directionality and anisotropy of the interaction are common in proteins, a better understanding of the role of patchiness for shear-induced aggregation is important for many biotechnological operations such as filtration, stirring, filling of containers, and pumping.

CPP 4.7 Mon 11:00 C 264

Unification of Lower and Upper Critical Solution Temperature Transitions in Aqueous Protein Solutions — •Nafisa Begam, Stefano Da Vela, Fajun Zhang, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen

Phase separation in aqueous protein solution is of primary interest in the field of many biological and chemical processes. In particular, phase separated protein solutions exhibiting lower/upper critical solution temperature (LCST/UCST) behavior have been of significant importance in the food and pharmaceutical industries. Based on theoretical calculations [1] and experimental observations, it is predicted that proteins can be designed with tunable LCST and UCST. Here, our goal is to experimentally design such aqueous protein system showing tunable LCST and UCST transitions. The UCST phase of β-Lactoglobulin - Yttrium Chloride (YCl_3) based aqueous systems at a salt concentration higher than a critical concentration, c*, has been already reported by our group [2]. However, we obtain evidence of LCST phase behavior of this system at a lower salt concentration but higher than c*. The solution becomes turbid at high temperature and clear at low temperature. Similar indication of the presence of both LCST and UCST phase behavior we get from the SAXS measurements on Bovine serum Albumin (BSA) - YCl_3 system. The findings of this study suggest a controllable dual phase of aqueous protein solution by tuning the ionic strength. [1] Jianguo Li et. al, *J. Chem. Phys.*, **128**, 235104, (2008) [2] F. Zhang et. al, *J. App. Crystal.*, **44**,755-762, (2011)

Invited Talk CPP 4.8 Mon 11:15 C 264

Reconfigurable colloidal structures — •Daniela J. Kraft — Soft Matter Physics, Huygens-Kamerlingh Onnes Laboratory, Leiden Institute of Physics, Leiden, The Netherlands

Reconfigurability is an essential feature of functional micro- and nanomachines. One way to realize reconfigurability is to introduce microscopic hinges, that is, elements that allow rotation while conserving the relative order of their arrangement. We have developed two experimental realizations of these pivotal elements on the colloidal length scale: I will first show how the deposition of oil droplets in colloidal aggregates lubricates the contact area and thereby enables and drives the reconfiguration into uniform, compact structures. Secondly, I will introduce colloidal particles with surface-mobile DNA linkers that enable the formation of strong and specific hinging bonds. I will describe how this bond mobility affects the self-assembly pathway and demonstrate the assembly of a variety of reconfigurable structures, such as floppy lattices, colloidal polymers and flexible colloidal molecules. These novel colloidal building blocks give access to a new class of materials with great potential in shape-shifting systems, actuators and colloidal robots.

CPP 4.9 Mon 11:45 C 264

Preparation of amphiphilic asymmetric patchy particles and their effect on emulsion properties — •Marco Rehosek, Akilavasan Jeganathan, and Frank Marlow — Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr/Germany

Asymmetric patchy particles (APPs) have two different functionalities on the opposing sides of such a micro- or nanoparticle. These functionalities can be of a magnetic, chemical, or optical nature. Here we study different chemical polarities. Amphiphilic APPs having hydrophobic and hydrophilic regions show interesting performance as emulsifying agent. This effect enhances the so-called Pickering stabilization resulting in a "breathable skin" at a liquid|liquid interface.

In this work, the preparation of amphiphilic APPs and their effect on emulsions is studied. Titania&organosilane APPs were prepared via a wax-masking-symmetry breaking step. The unmasked part was modified by vapor deposition. The effect of the APPs on emulsion stability and aging effects of APP-stabilized emulsions was studied qualitatively by liquid-phase-distribution measurements. For a deeper understanding, rheological properties of the emulsions were investigated. Viscosimetry gave information on stress-dependent viscosity effects, while oscillation measurements reveal the viscoelastic properties. Long-time measurements resulted in information on aging processes in the emulsion i.e. creaming, coalescence and Ostwald ripening.

CPP 4.10 Mon 12:00 C 264

On effective sphere models for self-diffusion of nonspherical particles — •Felix Roosen-Runge, Jin Suk Myung, Peter Schurtenberger, and Anna Stradner — Division of Physical Chemistry, Lund University, Sweden

Modeling diffusion of nonspherical particles presents an unsolved and considerable challenge, despite its importance for the understanding of crowding effects in biology and nanotechnology. A common approach is the mapping of nonspherical objects on effective spheres to subsequently approximate phenomena for nonspherical particles with the established predictions for spheres. Using hydrodynamic simulations, we show that this so-called effective sphere model fundamentally fails to represent the short-time self-diffusion of nonspherical particles even at low volume fractions and small to moderate nonsphericities. Based on analytical theory of hydrodynamic interactions, we discuss possible improvements for the modeling as well as the implications of our findings for studies employing effective spheres.

CPP 4.11 Mon 12:15 C 264

Ultrasoft colloids under pressure driven flow — •Deepika Deepika and Arash Nikoubashman — Institute of Physics, Johannes Gutenberg University, Staudingerweg 7, 55128 Mainz, Germany

Star-shaped polymers show a continuous change of properties from flexible linear chains to soft colloids, as the number of arms is increased. To investigate the effect of macromolecular architecture on the flow behavior, we employed computer simulations of single star polymers as well as of mixtures of star and linear polymers under dilute conditions. Hydrodynamic interactions were incorporated through the multi-particle collision dynamics (MPCD) technique, while a bead-spring model was used to describe the polymers. At rest, the polymers were distributed homogeneously in the slit channel, irrespective of the number of arms. Once flow was applied, however, we found that the stars migrated more and more towards the channel center as the number of arms increased and the polymers became more rigid. These findings are in contrast to previous findings for deformable vesicles, where the softer particles moved to the channel center. We surmise that the observed behavior for polymers is due to effective arm stretching and hydrodynamic repulsion with the channel walls. In the star-chain mixtures, we found a flow-induced separation between stars and chains, with the stars being in the center and the chains closer to the walls. The results from our study give valuable insights for designing microfluidic devices for separating particles based on their rigidity.

CPP 4.12 Mon 12:30 C 264

Control of physico-chemical properties of Pickering emulsions for catalysis — •Dmitrij Stehl[1], Tobias Pogrzeba[2], Lena Hohl[3], Yuri Lvov[4], Matthias Kraume[3], Reinhard Schomäcker[2], and Regine von Klitzing[1] — [1]Festkörperphysik, TU Darmstadt, Darmstadt, Deutschland — [2]Institut für Chemie, TU Berlin, Berlin, Deutschland — [3]Prozess- und Verfahrenstechnik, TU Berlin, Berlin, Deutschland — [4]Institute for Micromanufacturing, Lousiana Tech University, Lousiana, USA

Pickering-emulsions (PEs) are particle-stabilized emulsions. Different solid nanoparticles stabilize emulsion droplets against coalescence. Halloysite nanotubes (HNT) can be used as emulsifier. These particles are multiwall, inorganic tubes with negative charges at the outer surface and positive charges at the inner surface. The length of the HNTs in this study is 800 +- 200 nm and the outer diameter is 50 nm. HNTs adsorb laterally at the water/oil interface and the energy of detachment is several 10.000 kT. Due to the anisotropy of the HNT, the behavior of the nanotubes at the interface is different from spherical particles and the stability of the respective PE is higher which is studied in detail. The effect of different parameters on the structure of the PEs is studied, like HNT surface modification and energy input by the PE-fabrication, effect of HNT concentration, salt (NaCl) concentration and pH. In this study, the hydroformylation of long chain olefins (1-Dodecene) in PEs was used as a model system. The water phase contains the homogeneous Rh-catalyst and the oil phase (1-Dodecene) is simultaneous the reactant.

CPP 4.13 Mon 12:45 C 264

Crystal-fluid surface tension in the two dimensional binary hard disk mixture, a DFT study — •Shang-Chun Lin and Martin Oettel — Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany

Using fundamental measure theory, we investigate phase diagrams and crystal-fluid surface tensions in additive and nonadditive two-dimensional hard disk mixtures of small and large spheres with size ratio q. In the nonadditive case, the small disks act as ideal "polymeric" depletants (Asakura-Oosawa model) and the surface tension (for small q) shows a minimum with increasing small sphere concentration. We compared to the additive case, with an interface between fluid and crystals with substitutional disorder, and find a similar behavior (for small q). For larger q, the surface tension is almost constant upon adding the small spheres. In these investigations, the fluid-solid transitions were first-order due to the assumption of a periodic unit cell in the DFT calculations. We examine the possibility of relaxing this assumption and finding a hexatic phase in fundamental measure theory.

CPP 5: Polymer Networks and Elastomers I

Time: Monday 9:30–12:45 Location: PC 203

Invited Talk CPP 5.1 Mon 9:30 PC 203

Strain-controlled criticality governs the nonlinear mechanics of fibre networks — •Abhinav Sharma[1,2], Albert Licup[2], Karin Jansen[3,4], Robbie Rens[2], Michael Sheinman[2], Jordan Shivers[5], Jingchen Feng[5], Gijsje Koenderink[3], and Fred MacKintosh[2,5] — [1]Leibniz Institute for polymer research, Dresden — [2]Vrije Universiteit Amsterdam — [3]AMOLF, Amsterdam — [4]University of Manchester, UK — [5]Rice University, Houston, USA

Disordered fibrous networks are ubiquitous in nature as major structural components of living cells and tissues. The mechanical stability of networks generally depends on the degree of connectivity: only when the average number of connections between nodes exceeds the isostatic threshold are networks stable1. On increasing the connectivity through this point, such networks undergo a mechanical phase transition from a floppy to a rigid phase. However, even sub-isostatic networks become rigid when subjected to sufficiently large deformations. To study this strain-controlled transition, we perform a combination of computational modelling of fibre networks and experiments on networks of type I collagen fibres, which are crucial for the integrity of biological tissues. We show theoretically that the development of rigidity is characterized by a strain-controlled continuous phase transition with signatures of criticality. Our experiments demonstrate mechanical properties consistent with our model, including the predicted critical exponents.

CPP 5.2 Mon 10:00 PC 203

Rheology of cross-linked polymer networks — •Jakob Löber — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Polymer networks and gels may exhibit complex rheological behavior as e.g. an increase of the shear modulus in time known as rheological aging, shear rejuvenation, and a yield stress. I present a model for cross-linked polymer networks which treats the number of cross-links as a thermodynamic variable. This number may change due to a chemical reaction modeled as a rate equation, with a chemical equilibrium constant depending on mechanical deformations. Thus applying e.g. a large shear deformation affects the number of cross-links, leading to nonlinear threshold behavior reminiscent of shear rejuvenation and yield stress.

CPP 5.3 Mon 10:15 PC 203

Separation of entropy and energy elastic contributions and the strain induced crystallization during the deformation of rubber — •Konrad Schneider — Leibniz-IPF Dresden, Germany

Matrix-filler-interaction as well as strain induced crystallization (SIC) are main processes, responsible for the outstanding mechanical performance of natural rubber. By IR thermography combined with synchrotron x-ray diffraction it is possible to separate different mechanisms of deformation, reinforcement and failure in unfilled as well as filled rubber systems. Some recent measurements will be presented and discussed in detail.

CPP 5.4 Mon 10:30 PC 203

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

Using a highly efficient GPU version of the bond-fluctuation model, we study the elastic properties of end-linked 4-functional model networks where we can switch off either entanglements or both entanglements and excluded volume. With that we can separate the contribution of the connectivity and the topological constraints to the shear modulus and analyze them as a function of the strain in a simple shear deformation in our computer simulations. For the connectivity contribution, we take into account network defects, finite cyclic structures and the effect of excluded volume. The splitting of the contributions to the shear modulus from the connectivity and the entanglements is assumed in theory and it is checked explicitly with our simulation data. We estimate the entanglement degree of polymerization and compare its scaling with existing studies confirming the theoretical prediction, $N_\mathrm{e}(\phi) = N_\mathrm{e}(1)\,\phi^{1.3}$.

CPP 5.5 Mon 10:45 PC 203

The elasticity of phantom networks with cyclic and linear defects — •Michael Lang — Institut Theorie der Polymere, Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany

The resistor network analogy is used to compute the phantom modulus of realistic polymer networks containing finite cycles. We correct a recently published approach [1], connect with results on the distribution of cyclic defects, and generalize to networks of arbitrary junction functionality containing both cyclic and linear defects. It turns out that the impact of finite cyclic structures on rubber elasticity was previously [1] overestimated and that a consideration of the smallest dangling loops in combination with a precise estimate of conversion is sufficient in most cases for estimating the phantom modulus of the network.

[1] M. Zhong, R. Wang, K. Kawamoto, B. D. Olsen, J. A. Johnson. *Science*, 353:1264–1268, 2016.

15 min. break

CPP 5.6 Mon 11:15 PC 203

Network formation and dynamics in H-bonding telechelic polymers: competition between association time and structural relaxation — •Martin Tress[1], Kunyue Xing[1], Pengfei Cao[2], Shiwang Cheng[1], Tomonori Saito[2], Vladimir Novikov[1], and Alexei Sokolov[1,2] — [1]University of Tennessee Knoxville, Department of Chemistry, Knoxville, Tennessee, USA — [2]Oak Ridge National Lab, Chemical Sciences Division, Oak Ridge, Tennessee, USA

Reversible bonds between polymer chains can form supra-molecular networks which exhibit extraordinary mechanical properties. In fact, reversible bonds are a promising route to functional materials with self-healing properties. We study short telechelic polymers with H-bonding end-groups of different interaction strength and backbone flexibility. The glass transition temperature of flexible polydimethyl siloxanes (PDMS) does not vary with H-bond strength, but differs strongly from methyl-terminated PDMS. At the same time, Tg of the much stiffer telechelic polypropylene glycol (PPG) depends significantly on the H-bond strength. In contrast, viscosity strongly depends on the H-bond strength in the PDMS series while it remains almost the same in PPG with different end groups. Complementary measurements of shear modulus and dielectric relaxation indicate that these observations can be explained by competing lifetimes of supra-molecular associations and structural relaxations. Only if the association lifetime exceeds the characteristic segmental or chain relaxation time, the glass transition or viscosity will be affected by chain associations. Otherwise the chain end associations do not influence significantly Tg or viscosity.

CPP 5.7 Mon 11:30 PC 203

Molecular properties and growth conditions associated with PSS diffusion during annealing in polyelectrolyte multilayers — •Annkatrin Sill, Amir Azinfar, Sven Neuber, Peter Nestler, and Christiane A. Helm — Inst. f. Physics, Greifswald University, Germany

During annealing of polyelectrolyte multilayers in concentrated solutions (1 M NaCl) interdiffusion of polyelectrolytes occurs. We investigate the interdiffusion perpendicular to the substrate using neutron reflectivity and selectively deuterated polyanions (poly(styrene sulfoante), PSS). Multilayers formed at 10 mM consist of flatly adsorbed chains. The diffusion constant of PSS can be tuned by five orders of magnitude; it decreases exponentially with the degree of polymerization of PDADMA (poly(diallyldimethylammonium)). Multilayers formed at 100 mM NaCl consist of interdigitated chains. When the degree of polymerization of PDADMA exceeds the one of PSS, the diffusion constant drops suddenly by three orders of magnitude and remains low. Such sudden transitions are better known from network than from polymer theory.

CPP 5.8 Mon 11:45 PC 203

Application of the dynamic flocculation model for investigations of silica filled rubbers — •David Lockhorn and Manfred Klüppel — Deutsches Institut für Kautschuktechnologie e.V., Eupener Straße 33, D-30519 Hannover, Germany

The dynamic flocculation model (DFM) was introduced to describe the strong non-linear stress-strain behavior of filler reinforced rubbers. The model is able to describe stress-softening as well as hysteresis by a combination of well-established concepts for rubber elasticity and a micromechanical approach for the dynamic filler flocculation in strained rubbers. The stress value at a given strain leads back to an ongoing breakdown and reaggregation of filler clusters. Multihysteresis measurements of silica filled natural rubber (NR) and styrene-butadiene rubber (SBR) compounds will be described by the DFM and some of the physically meaningful parameters will be interpreted with respect to reinforcement in NR/Silica compounds. Besides this, the physicals as well as the modulus with increasing strain which is a measure for the Payne effect will be shown for the used model compounds. The results lead to the conclusion that there is a good coupling between silica and NR especially for the coupling agent silane as expected. But by looking at the Payne effect there is an unexpected high value for the coupling agent compounds in NR. This indicates that the micro-dispersion is not sufficient.

CPP 5.9 Mon 12:00 PC 203

Modeling magnetic elastomers as coatings with controllable hydrophobicity — •Pedro A. Sanchez[1], Elena Minina[1], Sofia S. Kantorovich[1,2], and Elena Yu. Kramarenko[3] — [1]Computational Physics, University of Vienna, Vienna, Austria — [2]Ural Federal University, Ekaterinburg, Russia — [3]Moscow State University, Moscow, Russia

Magnetic elastomers are hybrid materials consisting of a soft matrix of polymers with a high volume fraction of embedded magnetic micro- and/or nanoparticles. These materials are elastic enough to experience strong structural changes as a response to external magnetic fields. This makes them promising candidates for a broad range of applications.

One particularly interesting application of magnetic elastomers is their use as thin coatings that provide a fine control of the hydrophobicity of their free surface, as a consequence of the strong changes in its roughness induced by the application of proper external fields.

In this contribution we present a minimal computer simulation model of a magnetic elastomer thin coating that captures the dependence of its surface roughness on the elastic properties of the polymer matrix and the magnetic interactions. This modeling approach may contribute to the optimum design of these systems.

CPP 5.10 Mon 12:15 PC 203

FORC diagrams in different systems of magnetic elastomers studying by molecular dynamics simulations — •Alla Dobroserdova[1], Pedro A. Sanchez[2], and Sofia Kantorovich[1,2] — [1]Ural Federal University, Ekaterinburg, Russia — [2]University of Vienna, Vienna, Austria

Magnetic elastomers are the systems consisting of magnetic particles distributed in a nonmagnetic elastic matrix. We use the FORC (first-order reversal curves) diagrams to study how the matrix influences on internal magnetic interactions. We use the Molecular Dynamics Simulations to model the different systems. We consider fixed nonmagnetic particles which are connected with dipolar ones by elastic interactions. We study the systems with translational constraints only as well as the systems with translational and rotational constraints. The first step is to get the main hysteresis loop of this system in computer simulations (the direction and intensity of an external magnetic field are changing). After that we need to perform the computer simulations to obtain the first-order reversal curves. In the result, we have dependence of FORC diagrams on coercive and reversal fields. We use classical method [C. R. Pike et al., J. Appl. Phys. 85, 6660 (1999)] to get the FORC diagrams. The research was supported by the Ministry of Education and Science of the RF (project 3.1438.2017/4.6) and Austrian Science Fund (FWF, START-Project No. Y 627-N27).

CPP 5.11 Mon 12:30 PC 203

Marginally compact hyperbranched macromolecular trees — •Maxim Dolgushev — Laboratoire de Physique Théorique de la Matière Condensée, Université Pierre et Marie Curie, Paris, France

This contribution presents our recent studies [1,2] on fractal hyperbranched trees with a Gaussian chain statistics, which are marginally compact. Marginal compactness means that in the $d = 3$ dimensional space the average size R of the trees follows $N \sim R^3$ (where N is the molecular mass of the tree), and at the same time for their surface A the relation $A \sim N$ holds. We show that albeit the self-contact density ρ_c diverges for marginally compact objects logarithmically with the molecular weight N, this issue can be overcome by introducing linear spacers. Indeed, the spacers of length S yield a $log(N/S)/S^{1/2}$ behaviour, so that the strong decay with S bits rapidly the logarithmic divergence [1]. Another recipe for suppression of the self-contact density ρ_c is introduction of local stiffness [2].

[1] M. Dolgushev, J. P. Wittmer, A. Johner, O. Benzerara, H. Meyer, and J. Baschnagel, Soft Matter 13, 2499-2512 (2017).

[2] M. Dolgushev, A. L. Hauber, P. Pelagejcev, and J. P. Wittmer, Phys. Rev. E 96, 012501 (2017).

CPP 6: Magnetic nanoparticles (joint session MA/CPP)

Time: Monday 9:30–12:15 Location: H 0112

CPP 6.1 Mon 9:30 H 0112

Temperature dependence of the magnetic anisotropy of Pt/Co/Pt nanodots — •Stefan Freercks, Eva-Sophie Wilhelm, Carsten Thönnissen, Philipp Staeck, and Hans Peter Oepen — Center for Hybrid Nanostructures, Universität Hamburg, Germany

We use the anomalous Hall-effect to investigate the magnetization reversal of single Pt/Co/Pt nanodots (diameter <35nm, Co thickness< 1.5nm) with perpendicular magnetization. The dots are fabricated by electron beam lithography and ion milling out of thin multilayers[1]. Our technique allows for measuring from room temperature, where the nanodots are usually superparamagnetic, down to low temperatures, where the magnetization is blocked. Measuring the switching times, we find that the attempt frequencies given by the Néel-Arrhenius law are some orders of magnitude higher than the expected GHz regime. Simple considerations show that a temperature dependent anisotropy can very well explain such deviations, which gave the motivation for our investigation. We determined the anisotropy of the initial film and of nanodots as a function of temperature. The anisotropy shows a non-linear temperature dependence in films and dots, which proves our point that temperature effects cannot be neglected in the Néel-Arrhenius law. Furthermore, the temperature dependence varies for different nanodots. The latter variation reveals that generalizations in ensemble measurements have to be handled with care. Funding by DFG via SFB 668 is gratefully acknowledged. [1] A. Neumann et al. Nano Letters. 13, p2199-2203, (2013)

CPP 6.2 Mon 9:45 H 0112

Non-coherent reversal of magnetization in single Pt/Co/Pt nanodots with diameter below 100nm — •Eva-Sophie Wilhelm, Stefan Freercks, Philipp Staeck, Carsten Thönnissen, and Hans Peter Oepen — Center for Hybrid Nanostructures, Universität Hamburg, Germany

We investigate magnetization reversal behavior of single Pt/Co/Pt nanodots with a diameter of 35nm and a Co thickness of 1nm using anomalous Hall-effect magnetometry [1] at temperatures from 2.5K to 270K. The samples were fabricated from polycrystalline films by electron beam lithography and ion milling.

For nanodots with uniaxial anisotropy and a diameter below 100nm single domain behavior and coherent rotation reversal according to the Stoner-Wohlfahrt model is expected [2] [3]. However non-coherent switching with two jumps in the hysteresis is observed for some of the dots with out-of-plane magnetization at low temperatures. Comparison of the reversal of two different dots from the same film material and micromagnetic simulation using Mumax3 [4] gives hints that this finding is caused by different local magnetic properties of the initial films. The differences presumably originate from the distribution of grains of different crystal orientation in the nanodots. Funding by DFG via SFB 668 is gratefully acknowledged. [1] A. Neumann et al. Nano Letters. 13, p2199-2203, (2013) [2] A. Neumann, Ph.D thesis, Universität Hamburg, (2015) [3] E. C. Stoner and E. P. Wohlfarth, Philos. Trans. R. Soc. London, Ser. A 240, 599 (1948) [4] A. Vansteenkiste et al. AIP Advances 4 107133 (2014)

CPP 6.3 Mon 10:00 H 0112

Chemical and magnetic characterizations of ordered arrangements of magnetic nanoparticles — Asmaa Qdemat[1], Emmanuel Kentzinger[1], •Jin Xu[2], Giuseppe Portale[2], Marina Ganeva[3], Stefan Mattauch[3], Oleg Petracic[1], Ulrich Rücker[1], and Thomas Brückel[1] — [1]Jülich Centre for Neutron Science (JCNS) and Peter Grünberg Institute (PGI), JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Herzog-Wilhelm-Allee — [3]Jülich Centre for Neutron Science, Forschungszentrum Jülich, Outstation at MLZ, 85748 Garching, Germany

a.qdemat@fz-juelich.de Keywords: magnetic nanoparticles, grazing incidence small angle scattering, interparticle interactions

Magnetic nanoparticles and their assembly in highly ordered structures are principally interesting regarding the understanding of magnetic interactions and for future applications in information technology as e.g. magnetic data storage media or as material for spintronics.

The work to be presented focuses on the chemical and magnetic characterization of monolayer of CoFe2O4 nanoparticles on silicon substrate. Using Grazing Incidence Small Angle X-ray Scattering (GISAXS) we deduce the height profile of the nanoparticle, and a hexagonal ordering between those nanoparticles. Macroscopic magnetization measurement and polarized neutron reflectometry were used to deduce that the nanoparticles are weakly magnetized with respect to bulk CoFe2O4 and that a random in plane relative orientation of the nanoparticle magnetizations is obtained at zero applied field.

CPP 6.4 Mon 10:15 H 0112

Magnetic behavior of single- and polycrystalline nanoparticle superlattices — •Michael Smik[1], Genevieve Wilbs[1], Mauricio Cattaneo[1], Elisa Volkmann[1], Emmanuel Kentzinger[1], Stefan Mattauch[2], Ulrich Rücker[1], Oleg Petracic[1], and Thomas Brückel[1] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4), JARA-FIT, 52425 Jülich, GERMANY — [2]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ, Lichtenbergstr. 1, 85747 Garching, Germany

Magnetic nanoparticle (NP) assemblies form a novel type of artificial material which hold the promise to display properties that are not found in nature. We have succeeded in fabricating large 3D nanoparticle 'macrocrystals' using a novel centrifuge assisted sedimentation technique from commercially available spherical iron oxide NP. The assembly of polycrystalline samples up to 300 μm in size was possible, as well as a the realization of a nearly ideal macrocrystal. Using small angle x-ray scattering at our in-house instrument GALAXI the supercrystalline structure and quality of ordering could be characterized. The magnetic properties were investigated by a variety of magnetometric methods. Additional samples of nearly non-interacting NP were prepared to characterize the magnetic behavior of the individual NP. A comparision between the polycrystalline, single crystal and dispersed samples was performed. For a microscopic investigation of the magnetic ordering in the supercrystals, small angle neutron scattering was employed.

CPP 6.5 Mon 10:30 H 0112

Structural and magnetic characterization of Pd-decorated cobalt ferrite multifunctional nanoparticles — •Seyedeh Fatemeh Shams[1], Detlef Schmitz[2], Alevtina Smekhova[1], Nataliya Svechkina[1], Konrad Siemensmeyer[2], Amir Hossein Tavabi[3], Rafal E. Dunin-Borkowski[3], and Carolin Schmitz-Antoniak[1] — [1]Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Department for Quantum Phenomena in Novel Materials (EM-IQM), Helmholtz-Zentrum Berlin für Materialien und Energie, 12489 Berlin, Germany — [3]Ernst Ruska Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany

Pd-decorated CoFe2O4 multifunctional nanoparticles have been synthesized as a hybrid platform for simultaneous magnetic hyperthermia and photothermal therapeutic applications. Elemental and microstructural analyses have been conducted using TEM, HAADF STEM, EDS and ICP-OES. Experimental results confirm successful homogeneous Pd decoration on highly crystalline CoFe2O4 nanoparticles. Cations distributions, which have been inferred from XANES and XRD measurements, suggest the presence of considerable cation disorder, which increases with decreasing particle size for all of the samples. Magnetic properties of the nanoparticles have been investigated using XMCD and magnetometry. Intriguingly high-field XMCD reveals significantly enhanced total magnetic moments for both Fe and Co ions after Pd decoration. This substantially increased magnetization could lead to improved magnetic hyperthermia performance of the nanoparticles.

15 minutes break

CPP 6.6 Mon 11:00 H 0112

Distributed heat production in clusters of magnetic nanoparticles — Paola Torche[1], David Serantes[2], Sergiu Ruta[3], Roy Chantrell[3], and •Ondrej Hovorka[1] — [1]University of Southampton, Southampton, UK — [2]Universidade de Santiago de Compostela, Santiago de Compostela, Spain — [3]University of York, York, UK

We address the issue of quantifying the heat produced by a single magnetic nanoparticle (MP) embedded within an interacting MP cluster. This is relevant for MP hyperthermia considered as a modality for enhancing cancer therapies, where it becomes necessary to understand the distribution of heat production across a MP aggregate inside a living cell. The heat produced by MPs subject to time-varying external magnetic field can be determined from the area of the hysteresis loop. However, at the single-particle level of description, the magnetization of a MP undergoes a fluctuating stochastic process and the meaning of the hysteresis loop becomes ambiguous, as suggested also experimentally. It is then unclear how to quantify the heat production, especially if the interactions between MPs cannot be neglected.

We use the modern stochastic thermodynamics in combination with the Néel-Arrhenius theory of thermal relaxation of MPs to establish the relationship between the fluctuating work and entropy (heat) produced along the fluctuating magnetization trajectories of MPs. By considering the dipolar chains of MPs, we demonstrate a practical recipe for quantifying the heat produced by a single MP embedded within a chain, which then allows to map heat production distributions along the chains.

CPP 6.7 Mon 11:15 H 0112

Determination of individual magnetic moments of trapped superparamagnetic particles — •Ulrich Herr, Meng Li, Benjamin Riedmüller, Florian Ostermaier, and Sruthi Sunder — Institute of Micro- and Nanomaterials, Ulm University, Ulm

Superparamagnetic nanoparticles are used in lab-on-chip devices for detection of bio-analytes, drug delivery, or in hyperthermia. Many of these applications would benefit from precise knowledge of the magnetic moment of the individual nanoparticle, which may vary significantly between particles due to the statistical nature of the production process. We have recently demonstrated that individual magnetic particles (Dynabeads M-280 and MyOne T1) can be trapped over long times in a micro-conductor ring combined with an additional homogeneous magnetic field [1], which allows precise determination of a variety of microscopic parameters. Here we demonstrate that capturing more than one particle inside the trap can lead to stable arrangement of the particles inside the magnetic potential landscape of the trap. By measuring the average distance between the nanoparticles in a known trap potential we are able to determine the actual magnetic moment of the trapped nanoparticles, which can not easily be obtained in other ways.

[1] B. Riedmüller, F. Ostermaier, F., U. Herr, Trapping of superparamagnetic particles with a single current-conducting microring, IEEE Transactions on Magnetics 53 (2017) 5300706 DOI: 10.1109/TMAG.2017.2697722

CPP 6.8 Mon 11:30 H 0112

Studying the dynamic properties of pure cobalt ferrite nanoparticles and particles coated with silica in PEG-solution by magnetic AC-susceptometry — •Samira Webers[1], Melissa Hermes[2], Joachim Landers[1], Soma Salamon[1], Annette M. Schmidt[2], and Heiko Wende[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen — [2]Institute for Physical Chemistry, University of Cologne

The particle-matrix interaction in complex viscoeleastic composites is determined by the characteristic length scales between the magnetic particles and matrix structures. In this work, we study the particle-matrix interaction of a polyethylene glycol (PEG) polymer solution with tailored complexity and the mobility of two types of particles. Pure cobalt ferrite nanoparticles with a hydrodynamic radius of $r_{h,CFO} = 23.2$nm and cobalt ferrite particles coated with silica resulting in $r_{h,CFO@SiO_2} = 42.3$nm are dispersed in various concentrated polymer solutions with different PEG length. The dynamic properties of the two particle systems in various polymer solutions are characterized by magnetic AC-susceptometry. Here the Brownian relaxation of the particles in complex fluids are investigated in the frequency regime from 0.001 Hz -250 kHz and compared to the relaxation of the coated particles, where a shift of magnetic susceptibility spectra to lower frequencies is observed. The frequency dependent viscosity is also determined by temperature dependent magnetic AC measurements. This work is supported by the DFG-Priority Programme SPP1681.

CPP 6.9 Mon 11:45 H 0112

Intermediates and pH sensitive formation pathways of superparamagnetic Fe3O4 nanoparticles — •Mohammad Reza Ghazanfari[1], Seyedeh Fatemeh Shams[1,2], Mehrdad Kashefi[1], and Mahmoud Reza Jaafari[3] — [1]Department of Materials Science and Engineering, Ferdowsi University of Mashhad, 9177948974, Mashhad, Iran — [2]Peter Grünberg Institute (PGI-6), Jülich Research Centre, 52425 Jülich, Germany — [3]Biotechnology Research Center, Nanotechnology Research Center, School of Pharmacy, Mashhad University of Medical Sciences, Mashhad, Iran

In this work, by identification of reaction critical steps using study of pH variations trend and then investigation of structural, microstructural, and magnetic properties of each sample, the formation mechanism and reaction pathways of synthesis the nanoparticles of Fe3O4 (magnetite) phase by coprecipitation method were successfully recognized and presented. Based on the results, the formation mechanism and reaction pathways of magnetite nanoparticles synthesis during coprecipitation method can be explained in four critical steps as follows: (I) the formation of ferrous hydroxide phase from initial materials, (II) the transformation of ferrous hydroxide phase to lepidocrocite phase, (III) the transformation of lepidocrocite phase to goethite phase, and (IV) the transformation of goethite phase to magnetite target phase (or/and maghemite phase).

CPP 6.10 Mon 12:00 H 0112

Magnetic properties of shell-ferromagnetic precipitates in decomposed off-stoichiometric Ni-Mn-based Heusler alloys, studied by ferromagnetic resonance (FMR) — •F. Scheibel[1,3], D. Spoddig[1], R. Meckenstock[1], T. Gottschall[2,3], M. Fries[3], A. Çakir[4], M. Farle[1], O. Gutfleisch[3], and M. Acet[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, 47057 Duisburg, Germany — [2]High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [3]Institut für Materialwissenschaft FG Funktionale Materialien, Technische Universität Darmstadt, 64289 Darmstadt, Germany — [4]Department of Metallurgical and Materials Engineering, Muğla Sitki Koçman University, 48000 Mugla, Turkey

Off-stoichiometric $\mathrm{Ni_{50}Mn_{25-\mathit{y}}}X_y$ ($25 > y > 0$) Heusler alloys decompose into ferromagnetic (FM) $\mathrm{Ni_{50}Mn_{25}}X_{25}$ and antiferromagnetic $\mathrm{Ni_{50}Mn_{50}}$ components when annealed between 600 and 750 K [1]. In the case of $y = 5$ annealed at 650 K, shell-ferromagnetic $\mathrm{Ni_{50}Mn_{25}}X_{25}$ nano-precipitates of about 3 nm are formed. High-field FMR measurements up to 12 T verify the existence of a strong coupling of the shell of the precipitates with the surrounding $\mathrm{Ni_{50}Mn_{50}}$ matrix [2]. Magnetization measurements show a rotation of the shell-spins first above 5 T, while the core shows a soft FM behavior. The magnetic hysteresis is vertically shifted, which makes this material interesting for magnetic-field proof permanent memory application. Work supported by the Deutsche Forschungsgemeinschaft (SPP 1599).

[1] A. Çakir et al., Sci. Rep. 6 , 28931 (2016)

[2] F. Scheibel et al., AIP Adv. 7, 056425 (2017)

CPP 7: Biomaterials and Biopolymers (joint session BP/CPP)

Time: Monday 9:30–13:00 Location: H 1058

CPP 7.1 Mon 9:30 H 1058

PFG-NMR studies of ATP diffusion in PEG-DA hydrogels and aqueous solutions of PEG-DA polymers — •Günter Majer[1] and Alexander Southan[2] — [1]MPI für Intelligente Systeme, Heisenbergstr. 3, 70569 Stuttgart, Germany — [2]Institut für Grenzflächenverfahrenstechnik und Plasmatechnologie IGVP, Universität Stuttgart, Nobelstraße 12, 70569 Stuttgart, Germany

Adenosine triphosphate (ATP) is the major carrier of chemical energy in cells. The diffusion of ATP in hydrogels, which have a structural resemblance to the natural extracellular matrix, is therefore of great importance for understanding many biological processes. A powerful tool to determine the diffusion coefficients of ATP and other solutes directly, i.e. without the need for a fluorescent label and independent of any diffusion-model assumptions, is pulsed field gradient nuclear magnetic resonance (PFG-NMR). We present precise PFG-NMR measurements of ATP diffusion in PEG-DA hydrogels of various mesh sizes as well as in aqueous solutions of PEG-DA polymers, which are not cross-linked to a three-dimensional network. A major result of this work is that the diffusion coefficients are determined by the polymer volume fraction only, regardless of whether the polymers are cross-linked or not. Obviously, the ATP diffusion takes place only in the aqueous regions of the systems, with the volume fraction of the polymers, including a solvating water layer, being blocked for the ATP molecules. This modified obstruction model is most appropriate to correctly describe ATP diffusion in PEG-DA hydrogels.

CPP 7.2 Mon 9:45 H 1058

Ion and Molecule Transport Bulk and in Nanopores - a NMR study — •Sarah Schneider and Michael Vogel — TU Darmstadt Institut fuer Festkoerperphysik, Darmstadt, Germany

We analyze ion and molecule transport in aqueous salt solutions confined to nanopores as part of a project that aims to develop a new generation of nanosensors by combining biological and synthetic nanopores. While being highly selective and sensitive, biological ion channels lack the robustness for technological applications. Contrarily silica pores are well-proven in industrial and clinical environments, but possess inferior capabilities, e.g. no selectivity. A hybrid system would combine the favorable properties of both fields.

To optimize such pores, it is of strong interest to understand the influence of the confinement on the T-dependent ion and molecule transport inside. We vary the pore parameters systematically and study their effects on the dynamics by NMR. Using ^{1}H and ^{2}H NMR we can selectively investigate water dynamics whereas ^{7}Li and ^{23}Na NMR analyze the local and long-range dynamics of ionic species. Analyzing the local ion and water dynamics reveals a slowdown with increasing salt concentration, which may differ in bulk and confinement due to altered prospensity for crystallization. At a given concentration there is a slowdown in confinement with more heterogenious dynamics. Both can be explained by a slower layer at the pore walls and bulk-like dynamics in the pore center. Field-gradient NMR is applied to measure self-diffusion. The extent of the effect and the relation between short- and long-range dynamics depend on the confinement properties.

CPP 7.3 Mon 10:00 H 1058

Fluoridation of hydroxyapatite - time dependence and protective properties — •Thomas Faidt[1], Andreas Friedrichs[1], Christian Zeitz[1], Samuel Grandthyll[1], Michael Hans[2], Matthias Hannig[3], Frank Müller[1], and Karin Jacobs[1] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Functional Materials, Saarland University, Saarbrücken, Germany — [3]Clinic of Operative Dentistry, Periodontology and Preventive Dentistry, Saarland University Hospital, Homburg, Germany

The application of fluoride containing products to protect tooth enamel from caries is daily practice for many decades. However, to this day little is known about the time dependence of fluoride uptake in hydroxyapatite (HAP) which is the mineral component of human enamel. In our study, we used highly dense HAP pellet samples as a model system for the crystallites of tooth enamel. To investigate the time dependence of the fluoride uptake, samples were exposed to a fluoride solution (NaF, 500 ppm) for different times. XPS depth profiling revealed a saturation behavior both for the overall amount of fluoride taken up by the sample and for the thickness of the formed fluoridated layer. We found that the maximum thickness of the fluoridated layer is about 13 nm. To explore the efficacy of such an ultrathin layer as a protective shield against acid attacks, we used AFM to determine the etching rates of untreated and fluoridated HAP samples. In spite of very low fluoride concentrations in the fluoridated samples, our results show a strong reduction of the etching rate after fluoride treatment.

CPP 7.4 Mon 10:15 H 1058

Flexoelectricity in bones — •Fabian Vasquez-Sancho[1,2], Amir Abdollahi[3], Dragan Damjanovic[4], and Gustau Catalan[1,5] — [1]Institut Catala de Nanociencia i Nanotecnologia, Barcelona, Catalunya — [2]CICIMA, Universidad de Costa Rica, San Jose, Costa Rica — [3]Laboratori de Calcul Numeric, Universitat Politecnica de Catalunya, Barcelona, Catalunya — [4]Ecole Politechnique Federale de Lausanne (EPFL), Lausanne, Switzerland — [5]Institut Catala de Recerca i Estudis Avançats (ICREA), Barcelona, Catalunya

Bones have been known to generate electricity under pressure since Fukada and Yasuda's seminal measurement of bone piezoelectricity in 1957. This piezoelectricity is thought to be essential for bone's self-repair and remodelling properties, and its origin is attributed to the piezoelectricity of collagen (the main structural protein of bones). However, since the discovery of flexoelectricity, it is known that strain gradients can also generate voltages in materials of any symmetry. Here we have detected and quantified the flexoelectricity of bone and bone mineral (hydroxyapatite), and determined that flexoelectricity can account for bone's electrical response to inhomogeneous deformations. In addition, we have used the flexoelectric coefficient of hydroxyapatite to calculate the (flexo)electric fields generated by cracks in bone mineral. Crack-generated electricity has been found to be large enough to be able to induce osteocyte apoptosis and thus initiate the crack-healing process, indicating a central role of flexoelectricity in bone damage repair and remodelling.

Invited Talk CPP 7.5 Mon 10:30 H 1058

Light-based tools for investigating cell-ECM and cell-cell interactions — •Aranzazu del Campo — INM-Leibniz Institute for New Materials, Campus D2 2, 66123 Saarbrücken, Germany

Cells are able to sense and respond to biochemical and mechanical signals of their microenvironment. Despite impressive progress in the field of mechanotransduction, we still lack precise biophysical tools to dynamically regulate receptors and forces at the cell-ECM and cell-cell interfaces at molecular scale. In this context, novel tools based on phototriggers, light-driven molecular motors and optogenetics will be presented.

15 min. break

CPP 7.6 Mon 11:15 H 1058

Quantitative Prediction of Multivalent Ligand-Receptor Binding Affinities for Influenza, Cholera and Anthrax Inhibition — Susanne Liese[1,2] and •Roland R. Netz[1] — [1]Freie Universität Berlin, Fachbereich Physik — [2]University of Oslo, Department of Mathematics

Multivalency achieves strong, yet reversible binding by the simultaneous formation of multiple weak bonds. It is a key interaction principle in biology and promising for the synthesis of high-affinity inhibitors of pathogens. We present a model for the binding affinity of synthetic multivalent ligands onto multivalent receptors consisting of n receptor units arranged on a regular polygon. Ligands consist of a rigid polygonal core to which monovalent ligand units are attached via flexible linker polymers. The calculated binding affinities quantitatively agree with experimental studies for cholera toxin ($n=5$) and anthrax receptor ($n=7$) and allow to predict optimal core size and linker length. Maximal binding affinity is achieved for a core that matches the receptor size and for linkers that are slightly longer than the difference between receptor size and core size. We construct an enhancement diagram that quantifies the multivalent binding affinity compared to monovalent ligands. We conclude that multivalent ligands against influenza viral hemagglutinin ($n=3$), cholera toxin ($n=5$) and anthrax receptor ($n=7$) can outperform monovalent ligands only for a monovalent ligand affinity that exceeds a core-size dependent threshold value. Thus multivalent drug design needs to balance core size, linker length as well as monovalent ligand unit affinity.

CPP 7.7 Mon 11:30 H 1058

Are there knots in chromosomes? — Jonathan Siebert[1], Alexey Kivel[1], Tim Stevens[2], Ernest Laue[2], and •Peter Virnau[1] — [1]JGU Mainz, Institut für Physik — [2]Cambridge University, Department of Biochemistry

Recent developments have for the first time allowed the determination of three-dimensional structures of individual chromosomes and genomes in nuclei of single haploid mouse embryonic stem (ES) cells based on Hi-C chromosome conformation contact data. Although these first structures have a relatively low resolution, they provide the first experimental data that can be used to study chromosome and intact genome folding. Here we further analyze these structures and provide the first evidence that G1 phase chromosomes are knotted [1], consistent with the fact that plots of contact probability vs sequence separation show a power law dependence that is intermediate between that of a fractal globule and an equilibrium structure.

[1]J.T. Siebert et al., Are There Knots in Chromosomes?, Polymers 9:8 (2017)

CPP 7.8 Mon 11:45 H 1058

Small-angle X-ray scattering on gold nanoparticle-decorated DNA-origami nanostructures — •Kilian Frank[1,2], Caroline Hartl[1], Amelie Heuer-Jungemann[1], Tim Liedl[1], and Bert Nickel[1] — [1]Faculty of Physics and Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 München, Germany — [2]present address: Georg-August-Universität, Institute for X-ray Physics, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The DNA origami technique is a robust method for positioning guest molecules at the nanoscale, allowing for 3D crystalline assembly from monomeric building blocks. We report on synchrotron small-angle X-ray scattering (SAXS) experiments on DNA origami with guest gold nanoparticles. Geometric models were applied to investigate the particle placement and the lattice parameters of crystalline superstructures. In collaboration with Heinz Amenitsch (TU Graz) the model-free pair distance distribution function (PDDF) from the scattering data was analyzed. The PDDF reveals interparticle distances with nanometer resolution and is thus a valuable tool in the study of DNA-templated particle assemblies. The structure of a DNA-based lattice was confirmed to be rhombohedral with a spacing of 65 nm (T. Zhang, C. Hartl, S. Fischer, K. Frank, P. Nickels, A. Heuer-Jungemann, B. Nickel and T. Liedl. arXiv: 1706.06965). In situ SAXS confirmed previously found melting temperatures of the structures. These results help to optimize future designs of monomeric building blocks regarding lattice type and size.

CPP 7.9 Mon 12:00 H 1058

Magnetic collecting of malaria pigment crystals by magnetized thin films — •Szilvia Mucza[1], Tamas Prok[1], Agnes Orban[1], Adrienne Furedi[2], Peter Furjes[2], and Istvan Kezsmarki[1] — [1]Dept. of Physics, Budapest Uni. of Technology and Economics and MTA-BME Lendület Magneto-optical Spectroscopy Research Group, 1111 Budapest, HU — [2]Inst. of Technical Physics and Materials Science, Centre for Energy Research, HAS, 1121 Budapest, HU

Malaria pigment (hemozoin) crystals are the by-product of the hemoglobin metabolism and are unique indicators of the malaria infection. These micrometer-sized, needle-like, paramagnetic crystals have low crystal symmetry, thus show optical and magnetic anisotropy. Our group has been developing a malaria diagnostic device based on their linear dichroism and we aim to integrate a magnetic prefilter to increase the method's efficiency.

For this reason we started to investigate the behaviour of hemozoin crystals in their liquid suspension under magnetic field. To enhance the magnetic field gradient we designed micron-sized magnetizable periodic structures by lithography, and we observed the behaviour of synthetically prepared hemozoin crystals in liquid over these structures. We explained our observations theoretically, with the modeling of the magnetic properties near the surface of the periodic structure. We performed measurements under flow using an aligned microfluidic system to optimize different geometric parameters of magnetic structures.

CPP 7.10 Mon 12:15 H 1058

Fibers and glasses: the complex behavior of protein droplets — •Louise Jawerth[1,2], Elisabeth Fischer-Friedrich[3], Suropriya Saha[1], Anthony Hyman[2], and Frank Jülicher[1] — [1]MPI for the Physics of Complex Systems. Dresden — [2]MPI of Molecular Cell Biology and Genetics, Dresden — [3]Biotec, TU Dresden

Liquid-like protein droplets are intracellular compartments that segregate material without the use of a physical barrier such as a membrane. Such compartments are important in a wide array of biological processes ranging from embryonic development to pathological fiber formation during neurodegenerative disease. The existence of many of these compartments has been known for decades; however, only recently has it become clear that these compartments exhibit liquid-like properties. In this talk, I will discuss our efforts to characterize and quantify these new materials in vitro. I will preset our recent work on quantifying the mechanical properties of these droplets using a combination of active and passive microrheology. We find that these droplets are not simple liquids, but become increasingly elastic as the droplets age. This appears to be a universal behavior shared by many protein varieties that form droplets. Furthermore, this and other characteristics are strikingly similar to behaviors observed in glass-like materials suggesting that protein droplets are in fact not simple liquids but, rather, a type of glass.

CPP 7.11 Mon 12:30 H 1058

Light-driven biomolecule electrophoresis by asymmetric photochemistry — •Michael Kiess, Friederike Möller, and Dieter Braun — LMU Munich, Amalienstrasse 54, 80799 München, Germany

Ion and pH gradients across membranes are widespread in biology and are decisive for cell metabolism and signal transmission. We recreate such gradients in bulk water by local photolysis of photodissociable compounds. Focused light creates a non-equilibrium between photoproducts of different charges. Similar to pattern formation in biology, the differential diffusion of the photoproducts generates a radial electric field on a micrometer scale. Charged biomolecules move in this field through electrophoresis, which reaches a steady state within seconds in proportion to exp($-\mu/D\ \Phi$). The complete description and theoretical analysis of this phenomenon allows us to analyse and manipulate molecules in water. We call this effect photochemical microscale electrophoresis (PME) and use it as a fast, purely optical tool for the simultaneous determination of electrophoretic mobilities, diffusion coefficients and charges of biomolecules ($Q\propto\mu/D$) such as DNA and proteins as well as the quantification of binding probabilities. We expect that the presented photochemically induced, electrokinetic reaction-diffusion-migration system will be a versatile playground for further research. It can be a valuable tool for the investigation of electrokinetic effects and for the development of optical methods such as zeta potential measurements or isoelectric focusing. Furthermore, it is likely that the optically controlled interaction of electrical fields with pH and ion gradients may lead to a novel testbed for intracellular processes.

CPP 7.12 Mon 12:45 H 1058

Thermal gradients, a natural choice to support the origins of life — •Christof Mast[1], Lorenz Keil[1], Friederike Möller[1], Michael Kiess[1], Patrick Kudella[1], Mara Heinlein[1], Matthias Morasch[1], Hannes Mutschler[2], and Dieter Braun[1] — [1]LMU Munich, Amalienstrasse 54, 80799 München, Germany — [2]Max Planck Institute of Biochemistry, Am Klopferspitz 18, 82152 Martinsried, Germany

Life is a non-equilibrium system, which is nowadays maintained by a highly developed energy conversion machinery. Four billion years ago, other non-equilibrium mechanisms were needed to kick-start living processes. We propose ubiquitous heat fluxes as suitable driving force: Thermal gradients across water filled pores lead to a concurrent fluid convection and directed movement of dissolved charged molecules along the temperature difference. Combined, both effects accumulate the dissolved biomolecules in a length dependent manner. Oligonucleotides are pushed into a hydrogel phase, depending on their sequence and chirality: A mixture of strands with different sequence demixes into sequence-pure and homochiral hydrogels upon thermal accumulation, possibly selecting for interacting strands during the origin of life. The thermal non-equilibrium also creates and maintains a pH gradient over two units by the selective accumulation of charged buffer molecules, which shifts the local equilibrium in pH. In this system, early compartments of life may have cycled between different external pH conditions, implementing an important boundary condition for a primordial metabolism. [1] Keil et al. Nat Com, 2017, 10.1038/s41467-017-02065-3

CPP 8: 2D Materials (Symposium and Joint Session with HL and O): Session I (joint session DS/CPP/HL)

Time: Monday 9:30–13:15 Location: H 2032

CPP 8.1 Mon 9:30 H 2032

Graphene nanoribbon: electronic band structure, doping and Raman fingerprints — •Boris Senkovskiy[1], Dmitry Usachov[2], Alexander Fedorov[2,3], Gianni Profeta[4], Danny Haberer[5], Felix Fischer[5], and Alexander Grüneis[1] — [1]II. Institute of Physics, University of Cologne, Cologne, Germany — [2]St. Petersburg State University, St. Petersburg,Russia — [3]IFW-Dresden, Dresden, Germany — [4]Department of Physical and Chemical Sciences and SPIN-CNR, University of L'Aquila , Coppito, Italy — [5]Department of Chemistry, University of California at Berkeley, Berkeley, USA

We present the state-of-the-art studies of atomically precise graphene nanoribbons (GNRs) synthesized using on-surface assisted molecular assembly. Using angle-resolved photoemission spectroscopy (ARPES), we obtain the band structure of pristine and boron-doped armchair GNRs of N=7 carbon atoms width. ARPES maps in the full 2D momentum space visualize each sub-band of quasi-1D GNRs and allow to extract effective masses, charge carrier velocities and sub-band energy offsets. Vibration properties of GNRs are probed in-situ by ultra-high vacuum Raman setup. We show how the periodically incorporated boron atoms affect the band structure and the Raman-active modes of GNRs. Particularly, in doped nanoribbons the effective mass of charge carriers is $\sim$2 times smaller and the peculiar Raman modes are red-shifted and doubled regarding to the pristine system.

[1] Senkovskiy et al. Adv. Electron. Mater. 2017.
[2] Senkovskiy et al. Nano Lett., 2017.
[3] Senkovskiy et al. Phys. Status Solidi RRL, 2017.

CPP 8.2 Mon 9:45 H 2032

Valley spin lifetimes reaching 100 ns in monolayer $MoSe_2$ at room temperature — •Maximilian Heithoff, Manfred Ersfeld, Frank Volmer, Robin de Winter, Christoph Stampfer, and Bernd Beschoten — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany

We present time-resolved Kerr-rotation measurements on a monolayer of $MoSe_2$ revealing spin lifetimes up to 100 ns at room temperature. This extraordinary long-lived spin signal only weakly depends on temperature between 60 K and 300 K. At lower temperatures, it gets masked by an additional spin signal with significantly larger amplitude but shorter spin lifetimes reaching 8 ns. The latter spin signal exhibits a Kerr resonance which coincides with the photoluminescence spectrum from neutral and charged excitons showing that the spin dynamics at low temperatures are dominated by excitonic effects. In contrast, the long-lived spin signal at higher temperatures shows no resonance in the energy regime of the excitons. The absence of such resonance combined with the long spin lifetimes at room temperature is expected if the spin dynamics at elevated temperatures are not dominated by excitonic effects but by a polarization of resident holes, which is protected even at room temperature due to the large spin splitting in the valence bands of transition metal dichalcogenides.

CPP 8.3 Mon 10:00 H 2032

Ultra-high vacuum Raman spectroscopy of Cs doped monolayer graphene — •Martin Hell, Boris Senkovskiy, Joshua Hall, Thomas Michely, and Alexander Grüneis — II. Physikalische Institut, Universität zu Köln

We show that ultra-high vacuum (UHV) Raman spectroscopy is a valuable tool for in-situ characterization of epitaxial graphene on Ir(111) regarding strain, defects and doping level. We study the Cs doping induced changes in the Raman spectrum of epitaxial monolayer graphene for 2x2 and $\sqrt{3}$x$\sqrt{3}$ Cs adsorption geometries for exciting laser energies in a wide range (325nm to 633nm). The combined effects of lattice expansion and dynamic effects lead to characteristic changes in the Raman spectrum that allow us to identify the charge transfer and the electron-phonon coupling strength from the position, width and asymmetry of the G band Raman line. The electronic and structural characterization of Cs doped graphene is complemented by angle-resolved photoemission measurements and scanning tunneling microscopy on identically prepared samples. The high energy resolution of Raman ($\sim$1 wavenumber) allows for a precise determination of temperature induced strain of epitaxial graphene. Finally, we will show new results regarding the UHV Raman and luminescence characterization of transition metal dichalcogenides grown on graphene/Ir(111).

CPP 8.4 Mon 10:15 H 2032

Raman spectroscopy of misfit layer compound nanotubes from CrS_2 and TaS_2 — •Felix Kampmann[1,2], Dalit Stolovas[3], Leela S. Panchakarla[3], Gal Radovsky[3], Christian Thomsen[2], Reshef Tenne[3], and Janina Maultzsch[2] — [1]Institut für Festkörperphysik, TU Berlin, Berlin, Germany — [2]Institut für Physik der Kondensierten Materie, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany — [3]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, Israel

Misfit layer compounds (MLC) offer an interesting approach towards synthesis of novel one-dimensional nanostructures and two-dimensional materials. Understanding their structure and their physical properties has been subject to intense scientific research. The MLCs described by the formula MX-TX_2 consist of a transition metal dichalcogenide (TMD) layer TX_2 and an intercalation layer MX with distorted rocksalt structure. Here M denotes a metal, X is one of the elements S or Se, and T is of the group of transition metals.

In our study the TMD layer CrS_2 or TaS_2 is intercalated by either LaS-, CeS- or GdS- layers. Upon formation of the MLC charge transfer between the sublayers and deformation of the intercalation layer stabilize the otherwise metastable CrS_2. Due to the misfit between the sublayers in at least one direction and the seaming of dangling bonds at the rim atoms, the synthesis of nanotubes and -scrolls is favored. We investigate the vibrational properties of MLC nanotubes via Raman spectroscopy and discuss the results regarding previously published TEM methods.

CPP 8.5 Mon 10:30 H 2032

Photoluminescence study of MoS_2 monolayers integrated with photonic nanostructures — •Rajeshkumar Mupparapu[1], Tobias Bucher[1], Antony George[2], Frank Setzpfandt[1], Thomas Pertsch[1], Andrey Turchanin[2], and Isabelle Staude[1] — [1]Institute of Applied Physics, Abbe Center of Photonics, Friedrich Schiller University Jena, 07745 Jena, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany

Interaction of light with MoS_2 monolayers can be enhanced by integrating them with resonant nanostructures [1], and such interaction allows to manipulate their photoluminescence (PL) directionality and polarization. Here, we investigated the PL properties of MoS_2 monolayers integrated with resonant Silicon nanostructures [2] to explore the behavior of PL and valley polarization. Experiments performed on MoS_2-nanostructures reveal a significant PL enhancement [3], dominantly due to the local strain rather than Purcell enhancement. We further studied the valley polarization of MoS_2 flakes under different locally modified environments.

References:
[1]. S. Butun, *et al.*, Nano Lett., 2015, 15, 2700-2704.
[2]. M. Decker, I. Staude, J. Opt. 18, 103001 (2016).
[3]. T. Bucher, *et al.*, CLEO/Europe-EQEC 2017, Munich, EI-4.5, (2017).

CPP 8.6 Mon 10:45 H 2032

luminescence at defects in h-BN : excitons at stacking faults and single photon emitters — •Alberto Zobelli, Romain Bourrellier, Sophie Meuret, Michele Amato, Odile Stéphan, Luiz Tizei, and Mathieu Kociak — Laboratoire de Physique des Solides, University of Paris-Sud, CNRS, Orsay, France

h-BN is a promising material for optical application due to a strong exciton in the far UV and bright and stable defect emissions. Here we investigate the spatial localization at the nanometric scale of defects lines in this rich emission spectrum by employing an original cathodoluminescence system (nano-CL) integrated within a scanning transmission electron microscope. We show that high energy emissions are related to crystal folds leading to local changes of the layer stacking order which promote additional excitons. Furthermore, middle band gap emissions present a high spatial localization (~80 nm) and a typical zero-phonon line plus phonon replica spectroscopic signature, indicating a point defect origin. Finally, by combining our nano-CL system with an Hanbury Brown and Twiss (HBT) interferometer we identify a new bright and stable single photon emitter in the far UV.

CPP 8.7 Mon 11:00 H 2032

Density-functional perturbation theory for gated 2D heterostructures — •Thibault Sohier[1], Marco Gibertini[1], Nicola Marzari[1], Matteo Calandra[2], and Francesco Mauri[3] — [1]THEOS and MARVEL, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]IMPMC, CNRS, Université Pierre et Marie Curie, Paris, France — [3]Departimento di Fisica, Università di Roma La Sapienza, Roma, Italy

The ability to perform first-principles calculations of phonons and electron-phonon interactions in gated 2D heterostructures is crucial to the understanding and design of next-generation devices. Yet, standard methods relying on 3D periodic-boundary conditions fail to properly account for the consequences of dimensionality and the field-effect on electron-phonon physics. Here we present an implementation of density-functional perturbation theory using open boundary conditions adequate to the simulation of 2D systems, and with the possibility to add charged planes to emulate the doping of the slab via field-effect. We first illustrate the importance of working in the correct 2D framework with the study of long-wavelength phonons in polar materials, focusing on two mechanisms relevant for the performances of electronic devices: the Fröhlich interaction and the LO-TO splitting. Second, we address the consequences of the field-effect setup by looking at flexural phonons and their coupling to electrons in gated graphene. We observe that unlike isolated graphene, the coupling with flexural phonons in gated graphene is not forbidden by symmetry, but it is strongly suppressed by electronic screening.

15 min. break.

CPP 8.8 Mon 11:30 H 2032

Spectroscopic characterization of the silicene multi-layer phase on Ag(111) — •Dmytro Solonenko[1], Sandhya Chandola[2], Eugen Speiser[2], Norbert Esser[2], Dietrich R.T. Zahn[1], and Patrick Vogt[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V., 12489 Berlin, Germany

The formation of so-called "multi-layer silicene" has been suggested to form for supramonolayer Si coverages on Ag(111)[1], but its nature is still controversially discussed including silicene multi-layers, bilayers or Ag-mediated growth of bulk Si with a Ag-terminated $(\sqrt{3}\times\sqrt{3})$R30° reconstruction[2]. However, the experimental results which were shown so far do not allow an unequivocal assignment of this phase to any of the suggested structures. In order to retrieve the structural properties of this $(\sqrt{3}\times\sqrt{3})$R30° structure, we carried out an *in situ* Raman spectroscopy study varying the Si coverage (up to 10 monolayers). Our results show a unique spectral signature, which does not bear any resemblance to monolayer epitaxial silicene[3]. We compare the Raman results to those for the $(\sqrt{3}\times\sqrt{3})$R30° Ag/Si(111) system, yielding the similarities in terms of the overall number of spectral bands and their positions but also suggests fundamental differences, hinting towards the formation of a Si bilayer.

[1] Vogt, P., *et al.*, *Appl. Phys. Lett.* **104**, 021602 (2014). [2] Borensztein, Y., *et al.*, *Phys. Rev. B* **92**, 155407 (2015). [3] Solonenko, D., *et al.*, *2D Mat.* **4**, 015008 (2017).

CPP 8.9 Mon 11:45 H 2032

Frictional anisotropy of MoS2 studied with molecular dynamics simulations — •Victor Claerbout[1], Tomas Polcar[1,2], and Paolo Nicolini[1] — [1]Czech Technical University in Prague, Prague, Czech Republic — [2]nCATS, University of Southampton, Southampton, United Kingdom

Transition metal dichalcogenides are considered to be among the best solid lubricants due to their lamellar structure. Tribological research focused upon molybdenum disulfide has revealed its super low friction behavior [1]. However, a full understanding of the mechanism behind this behavior remains lacking. In this contribution we aim to elucidate the phenomena taking place at the nanoscale when two commensurate layers of molybdenum disulfide slide one atop of another. In particular, by means of molecular dynamics simulations, we studied the effect of sliding anisotropy [2] (i.e., the changing frictional behavior upon varying the sliding angle of two commensurate layers) on the energy dissipation due to friction. We simulated different sliding conditions (varying e.g. normal load, sliding speed and system temperature) in order to highlight their effect on the lubricating properties. These results will help on the one hand to identify the fundamental mechanisms that govern friction at an atomistic level, as well as providing guidelines for the design of novel layered materials with improved tribological properties.

[1] J.M. Martin et al., Phys. Rev. B, 48, 10583(R) (1993). [2] Onodera et al., J. Phys. Chem. B, 114, 15832 (2010).

CPP 8.10 Mon 12:00 H 2032

Structural changes and phase stability of Ti doped MoS$_2$ monolayers — •Andrea Silva, Tomas Polcar, Ondrej Hovorka, and Denis Kramer — Faculty of Engineering and Environment, University of Southampton, SO17 1BJ Southampton, United Kingdom

The discovery of graphene and its remarkable properties has renewed interest in inorganic materials and drawn attention to two-dimensional systems. Transition metal dichalcogenides (TMDs) have been known for decades in industry, but only recently their graphite-like layered structure has renewed academic interest. Quantum confinement in the monolayers yields different electronic properties compared to bulk counterparts. Moreover, TMDs are more chemically versatile than graphene, allowing easy functionalization of the layers [1]. Understanding the doping possibilities for TMDs is a key step in exploiting their potential.

In this study, we focus on the Ti doped MoS$_2$ TMD, a recently proposed new material with enhanced tribological properties [2].

In order to address the challenging task of determining the phase-stability of a new compound, we map energy landscapes obtained with DFT onto a cluster-expansion hamiltonian and iteratively search for low energy orderings of the atoms inside the given host. This methodology allows us to explore the Ti-Mo-S phase space and determine doping possibilities leading to stable phases of the form Ti$_x$Mo$_{1-x}$S$_2$, quantify miscibility gaps and thermodynamic competition with ternary oxides.

[1] M. Chhowalla *et al.*, Nat. Chem. 5, 263 (2013).

[2] A. Cammarata and T. Polcar, Inorg. Chem. 54, 5739 (2015).

CPP 8.11 Mon 12:15 H 2032

Resonance profiles of valley polarization in single-layer MoS$_2$ and MoSe$_2$ — •Hans Tornatzky[1], Roland Gillen[1,2], Anne-Marie Kaulitz[1], and Janina Maultzsch[1,2] — [1]Institut für Festkörperphysik, TU Berlin, Germany — [2]Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Transition metal dichalcogenides (TMDCs) attract a lot of interest due to their unique properties, such as the repeatedly investigated strong photoluminescence from the direct gap in few layered samples. Furthermore, TMDCs have recently become promising materials for spin- and valleytronics as circular polarized excitation leads to the generation of electron-hole-pairs with distinct spin at either K or $K*$ points in the Brillouin zone. However, questions remain unanswered about the mechanisms of the scattering processes.

In this talk we present photoluminescence measurements with different excitation energies on single-layer MoS$_2$ and MoSe$_2$ in order to examine the resonance behavior of the conservation of circular polarization in these TMDCs. We find that the circular polarization of the emitted light is conserved to 100 % in MoS$_2$ and 84 %/79 % (A/A^- peaks) in MoSe$_2$ close to resonance. The values for MoSe$_2$ surpass any previously reported value. However, in contrast to previous predictions, the degree of circular polarization decreases clearly at energies less than the 2 LA phonon energy above the resonance.

Our findings indicate that at least two competing processes underly the depolarization of the emission in single-layer transition metal dichalcogenides.

CPP 8.12 Mon 12:30 H 2032

Defect mediated phase transformation of two-dimensional 2H-MoTe2 to the distorted 1T'-MoTe2 — •Tibor Lehnert[1], Mahdi Ghorbani-Asl[2], Janis Köster[1], Hannu-Pekka Komsa[3], Arkady Krasheninnikov[2,3], and Ute Kaiser[1] — [1]Electron Microscopy Group of Materials Science, University of Ulm, Ulm 89081, Germany — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden 01328, Germany — [3]Department of Applied Physics, Aalto University, P.O. Box 11100, 00076 Aalto, Finland

We applied the newly developed Cc-and Cs-corrected SALVE (Sub-Angstrom Low-Voltage Electron Microscopy)[1] instrument, to study the dynamics of extended defects in single-layer 2H-MoTe2. In particular we report atom by atom on the transformation of an area in single-layer MoTe2 from the semiconducting 2H to the distorted and metallic 1T* phase, starting with a single vacancy line of missing Te atoms. We find that the size of the transformed area is defined by the length of the single vacancy line. First-principles calculations are performed to understand the transformation's driving forces.

[1] www.salve-project.de

CPP 8.13 Mon 12:45 H 2032

Excitonic transitions in heterostructured Mo and W transition metal dichalcogenides from first principles — •Roland Gillen and Janina Maultzsch — Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Novel two-dimensional materials from the group of layered transition metal dichalcogenides (TMDC) attract scientific interest for their unusual physical properties, such as their strong optical response. Two ways to tailor the electronic and optical properties are (i) the combination of different TMDCs to form lateral and stacked heterostructures and (ii) creation of alloys containing different metal or chalcogen atoms. Recent experiments have suggested long-lived interlayer excitons in stacked heterostructures, with spatial separation of electrons and holes across the layers, allowing for exploitation in solar cells.

Based on recent work [1,2], we show the theoretical absorption spectra of bilayer MoSe$_2$-WSe$_2$ and MoS$_2$-WSe$_2$ heterostructures from solution of the excitonic Bethe-Salpeter equation with GW quasiparticle corrections and inclusion of spin-orbit-coupling. In accordance with experimental observations, we find contributions related to interlayer excitons below the absorption onset of the monolayer materials. Our calculations allow us to estimate the binding energy of these electron-hole pairs to be on the order of 0.2 eV for both studied heterostructures. We will further show recent calculations of the absorption spectra of alloyed MoWS$_2$ materials.

[1] Gillen et al., IEEE JSTQE 23, 1 (2017), [2] Gillen et al., in preparation

CPP 8.14 Mon 13:00 H 2032

Suppression of inhomogeneous broadening of excitons and trions in encapsulated MoSe$_2$ monolayers — •Max Waldherr[1], Jacob Goddard[1], Nils Lundt[1], Sefaattin Tongay[2], Kenji Watanabe[3], Takashi Taniguchi[3], Sven Höfling[1,4], and Christian Schneider[1] — [1]Technische Physik, Physikalisches Institut and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]School for Engineering of Matter, Transport, and Energy, Arizona State University, Tempe, Arizona 85287, USA — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan — [4]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

Two-dimensional transition metal dichalcogenides offer a rich platform for the investigation of light-matter coupling effects due to unique effects such as spin-valley locking. In the monolayer limit the optical properties of these materials are highly sensitive to surface effects, hence the exciton and trion resonances undergo inhomogeneous broadening by surface impurities. We present a method to reduce the linewidth of these resonances involving encapsulation between two ultra-thin hexagonal boron nitride layers and thermal annealing in an argon-hydrogen atmosphere. With this technique inhomogeneous broadening is suppressed effectively which manifests in a Lorentzian line shape and improved optical quality. Moreover, the spectral weight of the exciton increases and the linewidths of the exciton and trion reduce to 2.9 and 2.4 meV, respectively.

CPP 9: Active Matter I (joint session DY/CPP/BP)

Time: Monday 10:00–13:15 Location: BH-N 243

CPP 9.1 Mon 10:00 BH-N 243

Dynamics of sedimenting active particles — •Jérémy Vachier and Marco G. Mazza — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

The collective motion of active particles has attracted enormous interest on account of the technological applications of artificial and biological particles. Even in the simple case of a dilute suspension solely subject to gravity, active particles show interesting behavior. While theoretical studies have addressed this problem with effective theories, a full time-dependent solution of the sedimentation problem has been neglected. Here, we present an analytical solution of the Fokker–Planck equation for the stochastic process which allows us to describe the full dynamics of active particles in three dimensions under an external force. Our results are supported by numerical calculations in which weak hydrodynamics interactions are approximated. We address three cases: active particle under gravity, confinement by reflecting barriers, and the effect of the activity of the particles on their collective motion. Finally, we compare our results with experiments and find a very good agreement.

CPP 9.2 Mon 10:15 BH-N 243

Active systems learning at the microscale — •Santiago Muiños-Landin[1], Keyan Ghazi-Zahedi[2], and Frank Cichos[1] — [1]Molecular Nanophotonics. University of Leipzig. Institut for Experimental Physics I — [2]Information Theory of Cognitive Systems, Max Planck Institute for Mathematics in the Sciences

Living organisms are able to sense and process information about the environment they live in. They are also able to update this information in order to contruct solutions for real life problems such as finding food or avoiding danger. This active adaption process that in the long run drives the evolution of species is the result of a short time scale evolution of the knowledge of an organism that we know as learning. At the microscale the learning is hampered by stochasticity given that the intrinsic Brownian noise makes critical to build a feedback between stimulus and action. Here, we present a system based on a self-themophoretic microswimmer that allows the application of artifical intelligence algorithms at the microscale. Using reinforcement learning we show that even under noise conditions a system is able to learn how to optimize a simple navigation task. We study the influence of noise and the situation where multiple agents can share information to carry out specific tasks. This way we show how adaptation and intelligent collective behavior can be studied in artificial microswimmers systems.

CPP 9.3 Mon 10:30 BH-N 243

Collective rotations of active particles interacting with obstacles — •Zahra Mokhtari[1], Timo Aspelmeier[2], and Annette Zippelius[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany — [2]Institut für Mathematische Stochastik, Georg-August-Universität Göttingen, Germany

We study the motion of active particles in the presence of static obstacles. We observe accumulation and crystallization of active particles around the obstacles which serve as nucleation sites, a phenomenon that is expected due to the known absorption of active particles at solid boundaries. In the limit of high activity, the crystals start to rotate spontaneously around the obstacle, resembling a rotating rigid body. We explain the occurrence of such rotations through the enhanced attraction of particles to the cluster whose orientation points along its rotational velocity as compared to those whose orientation points in the opposite direction.

CPP 9.4 Mon 10:45 BH-N 243

Collective dynamics of squirmers confined to a surface by strong gravity — •Jan-Timm Kuhr, Felix Rühle, Johannes Blaschke, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Hardenberg Str. 36, 10623 Berlin, Germany

External fields acting on microswimmers are of paramount importance for collective phenomena like bioconvection. In previous work we explored the individual [1] and collective [2] dynamics of squirmer model swimmers under moderate gravity by MPCD simulations. Here, we turn to strong gravity, where microswimmers form a single layer at the bottom surface, while interacting hydrodynamically in 3D.

We find various intriguing phenomena depending on the swimmer type (neutral, pusher, and puller) and area density: Formation of pairs, chains and other metastable bound states, but also collective swarming parallel to the surface.

Neutral squirmers at low area densities repel each other by their self-generated flow fields and thereby arrange in strongly disturbed hexagonal lattices reminiscent of 2D crystals subject to intense fluctuations. For higher densities attractive interactions become important and give rise to pair and chain formation. We characterize these distinct emergent states, compare to melting of 2D colloids, and explore the flow fields, which create hexagonal lattices.

[1] F. Rühle *et al.*, accepted at New J. Phys.
[2] J.-T. Kuhr, J. Blaschke, F. Rühle, and H. Stark, Soft Matter **13**, 7548 (2017).

CPP 9.5 Mon 11:00 BH-N 243

Learning agents as a model for collective motion — •Katja Ried[1], Thomas Müller[2], and Hans J. Briegel[1,2] — [1]Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 21a, 6020 Innsbruck, Austria — [2]Department of Philosophy, University of Konstanz, 78457 Konstanz, Germany

Watching a swarm of fish, birds or insects is mesmerizing, and it inevitably makes one wonder how countless independent individuals can form such a perfectly coordinated whole. A number of theoretical models attempt to answer this question by studying the collective dynamics that arise when individuals interact according to certain rules. However, these rules are often simply postulated ad hoc, and individuals are modelled as featureless points carrying them out. Naturally, such models are unlikely to provide an accurate - or even plausible - account of the individual-level behaviour that ultimately drives the swarm.

I will present a different Ansatz to this problem, wherein individuals are considered as full-fledged agents: distinct entities that can perceive certain (reasonable) features of their surroundings, endowed with a stable internal mechanism for processing these perceptions and deciding how to respond, and capable of modifying these responses as a function of their personal experience. I will illustrate this Ansatz with the example of locusts marching in a one-dimensional arena and discuss what insights agent-based models can offer to the study of collective motion.

15 min. break

CPP 9.6 Mon 11:30 BH-N 243

Localized States in an Active Phase-Field-Crystal Model — •Lukas Ophaus, Johannes Kirchner, Svetlana Gurevich, and Uwe Thiele — Institut für Theoretische Physik, WWU, Münster, Germany

The Phase-Field-Crystal (PFC) model provides a simple microscopic description of the thermodynamic transition from a fluid to a crystalline state [1]. The model can be combined with the Toner-Tu theory for self-propelled particles to obtain a model for crystallization (swarm formation) in active systems [2]. Within the resulting active PFC model, resting and traveling crystals can be identified. In the linear regime, we give analytical expressions for the transitions from the liquid state to both types of crystals. In addition, we provide a general semi-analytical criterion for the onset of motion in the nonlinear regime, that corresponds to a drift-pitchfork bifurcation. Like the passive PFC model [3], the active version describes a variety of localized states (LS) besides spatially extended crystals. In the spatially one-dimensional case we explore how the bifurcation structure (slanted homoclinic snaking) is amended by activity. Numerical continuation is applied to follow resting and traveling LS while varying the activity and mean concentration. A fold continuation allows us to determine the area of existence of different states in a two parameter plane. Finally, we look into the scattering behavior of LS through numerical time simulation. [1] M.J. Robbins et al., PRE 85, 061408 (2012). [2] A.M. Menzel and H. Löwen, PRL 110, 055702 (2013). [3] U. Thiele et al., PRE 87, 042915 (2013)

CPP 9.7 Mon 11:45 BH-N 243

Turbulence and pattern formation in a minimal model for active fluids — •Martin James[1], Wouter Bos[2], and Michael Wilczek[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]LMFA, CNRS, Ècole Centrale de Lyon, France

Continuum theories of active fluids display a fascinating range of dynamical states, including stationary patterns and turbulent phases. While the former can be tackled with classical pattern formation theory, the spatio-temporal disorder of active turbulence calls for a statistical description. In this presentation, new results on turbulence and pattern formation in a minimal continuum model for active fluids, which has been recently proposed by Wensink et al. [PNAS 109(36):14308 (2012)], will be discussed. Adopting techniques from turbulence theory, we establish a quantitative description of correlation functions and spectra for active turbulence. We furthermore report on a novel type of turbulence-driven pattern formation far beyond linear onset: the emergence of a dynamic vortex lattice state after an extended turbulent transient, which can only be explained taking into account turbulent energy transfer across scales.

CPP 9.8 Mon 12:00 BH-N 243

Emergence of phytoplankton patchiness at small scales in mild turbulence — Rebekka E. Breier, Cristian C. Lalescu, Michael Wilczek, and •Marco G. Mazza — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Faßberg 17, 37077 Göttingen

Phytoplankton often encounter turbulence in their habitat. As most toxic phytoplankton species are motile, resolving the interplay of motility and turbulence has fundamental repercussions on our understanding of their own ecology and of the entire ecosystems they inhabit. The spatial distribution of motile phytoplankton cells exhibits patchiness at distances of decimeter to millimeter scale for numerous species with different motility strategies. The explanation of this general phenomenon remains challenging. Furthermore, hydrodynamic cell-cell interactions, which grow more relevant as the density in the patches increases, have been so far ignored. Here, we combine particle simulations and continuum theory to study the emergence of patchiness in motile microorganisms in three dimensions. By addressing the combined effect of turbulent flow conditions, and spatial correlations in the particle positions, we uncover a general mechanism: when motility allows cells to cross the fluid streamlines, the typical length scale associated to the small-scale turbulence selects a characteristic cell-cell interactions scale where strong patches form. Our results shed light on the dynamical characteristics necessary for the formation of patchiness, and complement current efforts to unravel planktonic ecological interactions.

CPP 9.9 Mon 12:15 BH-N 243

Critical behavior of active Brownian particles — Jonathan Tammo Siebert, •Florian Dittrich, Friederike Schmid, Kurt Binder, Thomas Speck, and Peter Virnau — Johannes Gutenberg University Mainz, Department of Physics, 55122 Mainz

We propose an improved block-density distribution method, which allows us to determine accurately the critical point of two dimensional active Brownian particles at $\mathrm{Pe}_{\mathrm{cr}} = 40(2)$, $\phi_{\mathrm{cr}} = 0.597(3)$. Based on this estimate we study the corresponding critical exponents β, γ/ν, and ν. Our results are incompatible with the 2D-Ising universality class, thus raising the fascinating question whether there exists a non-equilibrium universality class.

CPP 9.10 Mon 12:30 BH-N 243

Pattern Formation and Synchronization of Disk-Shaped Circle Swimmers — •Guo-Jun Liao and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

We computationally study a generic model of disk-shaped active Brownian particles using Brownian dynamics simulation. Each particle is driven both by constant propulsion force and torque. We investigate how these two distinct propulsions combine to influence the macroscopic structure of a colloidal system. In the regime of small propulsion torque, the active colloids exhibit motility-induced clustering [1]. As the propulsion torque becomes comparable to thermal energy, the clustering phenomenon is drastically suppressed. Moreover, although all particles are intrinsically assigned to rotate counterclockwise, a novel state of clockwise vortices emerges at an optimal value of propulsion torque. We introduce a gear argument to capture the underlying mechanism of such vortices. To obtain deeper insight into the interplay between active motion and particle alignment, an additional polar interaction is then incorporated into our model. With increasing strength and range of the polar interaction, synchronization behavior is observed. Our model bears some similarity with the Kuramoto model [2], in which oscillators are actively moving over time.

[1] I. Buttinoni *et al.*, Phys. Rev. Lett. **110**, 238301 (2013)
[2] Y. Kuramoto, *Chemical Oscillations, Waves, and Turbulence*, (Springer, Berlin, 1984).

CPP 9.11 Mon 12:45 BH-N 243

Pair Creation in Insect Swarms — •Dan Gorbonos and Nir

Gov — Weizmann Institute, Rehovot, Israel

The macroscopic emergent behavior of social animal groups is thought to arise from the local interactions between individuals. We proposed a model of acoustic interaction within insect swarms that resemble gravitational attraction. Unlike gravity, the interactions between the insects are adaptive. Sensory mechanisms in biology, from cells to humans, have the property of adaptivity, whereby the sensitivity of the signal produced by the sensor is adapted to the overall amplitude of the signal. Adaptivity reduces the sensitivity in the presence of strong background stimulus, while increasing it when the background is weak. We find that in particular adaptivity is responsible for pairwise interaction that are characterized by higher-frequency nearly harmonic oscillations conducted by two synchronized insects. By comparison, the capture of pairs under normal gravity is extremely rare. We show that such pairs are created in simulations of the "adaptive gravity" model and compare them with pairs that were found in measurements of laboratory midge swarms. In addition we show similarities in density distributions between the simulations and laboratory measurements.

CPP 9.12 Mon 13:00 BH-N 243

Dynamically Generated Patterns in Dense Suspensions of Active Filaments — •Prathyusha Kokkoorakunnel Ramankutty[1], Silke Henkes[2], and Rastko Sknepnek[3] — [1]Max Planck Institute of Physics of Complex Systems, Dresden Germany — [2]University of Aberdeen, United Kingdom — [3]University of Dundee, United Kingdom

We use Langevin dynamics simulations to study dynamical behaviour of a dense planar layer of active semi-flexible filaments. Using the strength of active force and the thermal persistence length as parameters, we map a detailed phase diagram and identify several non-equilibrium phases in this system. In addition to a slowly flowing melt phase, we observe that for sufficiently high activity, collective flow accompanied by signatures of local polar and nematic order appears in the system. This state is also characterised by strong density fluctuations. Furthermore, we identify an activity- driven cross-over from this state of coherently flowing bundles of filaments to a phase with no global flow, formed by individual filaments coiled into rotating spirals. This suggests a mechanism where the system responds to activity by changing the shape of active agents, an effect with no analog in systems of active particles without internal degrees of freedom

CPP 10: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials I (joint session O/MM/DS/TT/CPP)

Exploring, understanding, and describing materials with strong electronic Coulomb correlations remain among the big challenges of modern condensed matter physics. Correlated materials are characterized by an extreme sensitivity to external probes such as pressure or temperature, and slight changes in composition, constraints during the growth process (e.g. by heterostructuring) or off-stoechiometries can significantly alter their properties. While the invited lectures will have a focus on correlated electron materials, the symposium will cover the general field of computational materials science and electronic-structure theory.

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Time: Monday 10:30–13:00 Location: HL 001

CPP 10.1 Mon 10:30 HL 001

How Derivative Discontinuities in the Energy Yield Interatomic Steps in the Exact Kohn-Sham Potential of Density-Functional Theory — •Eli Kraisler[1], Matthew J. P. Hodgson[1], Axel Schild[2], and Eberhard K.U. Gross[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale), Germany — [2]Laboratorium für Physikalische Chemie, ETH Zürich, Switzerland — [3]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Israel

Accurate density-functional calculations hinge on reliable approximations to the unknown exchange-correlation (xc) potential. The most popular approximations usually lack features of the exact xc potential that are important for an accurate prediction of the fundamental gap and the distribution of charge in complex systems. Two principal features in this regard are the spatially uniform shift in the potential, as the number of electrons infinitesimally surpasses an integer, and the spatial steps that form, e.g., between the atoms of stretched molecules. Although both aforementioned concepts are well-known, the exact relationship between them remained unclear. In this talk, we establish this relationship and introduce a new concept: the charge-transfer derivative discontinuity, Δ^{CT}. By numerically solving the many-electron Schrödinger equation, we extract the exact Kohn-Sham potential and directly observe its features, particularly the spatial interatomic steps. For the first time, spatial steps in the exact xc potential of a full configuration-interaction (FCI) calculation of a molecule are presented in three dimensions.

CPP 10.2 Mon 10:45 HL 001

Steps in the exact Kohn-Sham potential of ensemble density-functional theory for excited states and their relation to the derivative discontinuity — •Matthew J. P. Hodgson[1], Eli Kraisler[1], Michael T. Entwistle[2], Axel Schild[3], and Eberhard K. U. Gross[1,4] — [1]MPI für Mikrostrukturphysik, D-06120 Halle, Germany — [2]Dep. of Physics, Uni. of York, Heslington, YO10 5DD, UK — [3]Lab. für Physikalische Chemie, ETH Zürich, 8093, Switzerland — [4]Fritz Haber Center for Molecular Dynamics, The Hebrew University of Jerusalem, 91904, Israel

An accurate approximation to the exchange-correlation (xc) part of the Kohn-Sham (KS) potential is essential for any density-functional calculation. Understanding the behaviour of the exact xc potential and developing improved approximations to it are crucial. The focus of calculations within density functional theory is usually on the ground state. However, knowledge of how the system responds to an excitation is important. In this talk we present the exact KS potential of an ensemble of the ground state and the first excited state of a 1D diatomic molecule. For this system, upon excitation, a small amount of charge transfers from one atom to the other. In the corresponding exact ensemble xc potential we find two plateaus: one that forms around the nucleus of the acceptor atom, associated with the derivative discontinuity of that atom, and another that forms around the donor atom and corresponds to a new phenomenon which we term the 'charge-transfer derivative discontinuity'.

CPP 10.3 Mon 11:00 HL 001

Koopmans-compliant functionals: A reliable and efficient tool for the prediction of spectroscopic quantities — •Nicola Colonna[1], Ngoc Linh Nguyen[1], Andrea Ferretti[2], and Nicola Marzari[1] — [1]THEOS and MARVEL, EPFL, Lausanne, Switzerland — [2]Centro S3, CNR-Istituto Nanoscienze, Modena, Italy

Commonly used approximate density functionals produce total energies that do not exhibit the expected piecewise-linear behavior as a function of the particle number, leading to a discrepancy between total and partial electron removal/addition energies and poor predictive capabilities of ionization potentials. Koopmans-compliant functionals enforce a generalized criterion of piecewise linearity in the energy of any approximate density functional with respect to the partial removal/addition of an electron - i.e., with respect to charged excitations - from/to any orbital of the system. When used to purify approximate density functionals, Koopmans' corrections lead to orbital-density dependent functionals and potentials that are able to deliver accurate spectroscopic properties. As an example, ionization potentials of a large set of molecules (the GW100 test set), photoemission spectra of organic donors and acceptors and band gaps of 35 semiconductors and insulators are presented, showing very good agreement with experiment or higher-order theories. Being this a functional framework, the straightforward advantages are that forces and other derivatives are also readily accessible, that the computational costs are much reduced, and the numerical parameters are those typical of DFT calculations.

CPP 10.4 Mon 11:15 HL 001

Selfconsitent density embedding - a new class of functionals for DFT — •Uliana Mordovina[1], Teresa E. Reinhard[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

We propose a new technique to find functionals for density functional theory (DFT) in an ab-initio fashion. This technique origins in the recently developed density-matrix embedding theory (DMET) [1]. DMET is a quantum-in-quantum embedding method, which is based on finding a projection between the high-dimensional wave function of the full system and a lower-dimensional wavefunction living in the active space of the embedded system, which is then solved exactly. In the original DMET scope, the projection is improved via optimization of the reduced one-body density matrix. We replace this optimization by a density inversion, exploiting the one-to-one mapping between electronic density and Kohn-Sham potential.

The proposed density-embedding scheme serves as functional in DFT, which, unlike in usual DFT, can be systematically improved by increasing the size of the active space.

We show convergence toward exact results for 1D systems as well as results for 2D systems.

[1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012)

CPP 10.5 Mon 11:30 HL 001

Pressure dependence of the effective screened Coulomb interactions in transition metal monoxides — •Swarup Kumar Panda[1], Hong Jiang[2], and Silke Biermann[1,3] — [1]Centre de Physique Théorique, Ecole Polytechnique, France — [2]College of Chemistry and Molecular Engineering, Peking University, China — [3]Collège de France, Paris, France

In transition metal compounds, the magnitudes of the effective Coulomb interaction parameters (Hubbard U) and their pressure dependence are of utmost importance in any realistic many-body simulations for describing their pressure driven insulator-metal transition. One of the powerful methods for calculating the Hubbard U from first principles is based on linear response theory within the constrained random-phase approximation (cRPA) [1], which provides the full U matrix including off-site elements and its frequency dependence. In this presentation, we apply this method (in its implementation into the Wien2k code [2]) to the transition metal monoxides (FeO, CoO, NiO, and CuO) [3]. Although the pressure induced changes in the bare Coulomb interactions are negligible, the effective screened U grows monotonically with increasing pressure for all of the above monoxides. Finally, I will argue that neither the pressure dependence nor the frequency dependence of U should be ignored in a reliable theoretical description of correlated oxides.

References: [1] Aryasetiawan et al., PRB 70, 195104 (2004) [2] Vaugier et al., PRB 86, 165105 (2012) [3] Panda et al., PRB 96, 045137 (2017)

CPP 10.6 Mon 11:45 HL 001

Self-Interaction Corrected SCAN for Molecules: All-Electron Implementation with Numerical Atom-Centered Basis Functions — •Sheng Bi, Igor Ying Zhang, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

The self-interaction error (SIE) is a well-known problem in all semilocal density-functional approximations (DFAs), including the recently proposed "strongly constrained and appropriately normed" (SCAN) functional [1]. The so-called self-consistent Fermi-orbital SIC (FSIC) algorithm proposed by Pederson *et al.* [2] shows promising potential to eliminate the self-interaction error in semilocal approximations, which has been demonstrated for the local-spin-density approximation (LSDA) in a study of molecules.

We present an all-electron implementation of the self-consistent FSIC approach on the SCAN method [1]. Beside a systematic benchmark with respect to a selected molecular test set, we examine the performance of FSIC-SCAN in predicting the geometry of Pentacene, which is a well-documented challenge for standard semilocal DFAs [3]. Finally, we briefly discuss our ongoing work concerned with the implementation of the all-electron FSIC-SCAN approach for solids.

[1] J. Sun, A. Ruzsinszky, and J. P. Perdew, *Phys. Rev. Lett.* **115**, 036402 (2015).

[2] M. R. Pederson and T. Baruah, *Advances In Atomic, Molecular, and Optical Physics* **64**, 153 (2015).

[3] M. R. Pederson, T. Baruah, D. you Kao, and L. Basurto, *The Journal of Chemical Physics* **144**, 164117 (2016).

CPP 10.7 Mon 12:00 HL 001

Progress in Fermi-Löwdin orbital self-interaction correction to DFT — •Torsten Hahn[1], Sebastian Schwalbe[1], Simon Liebing[1], Mark Pederson[2], and Jens Kortus[1] — [1]TU Freiberg, Institute for Theoretical Physics, Germany — [2]Johns Hopkins University, Department of Chemistry, USA

The accuracy of density functional theory (DFT) calculations is limited by the so called self-interaction error [1]. The recently proposed Fermi-Löwdin orbital based method [2,3,4] for self-interaction correction (FLO-SIC) is a unitary invariant and size extensive approach to overcome this error. We present the current state of the method and discuss the performance of FLO-SIC DFT applied to atoms and molecules in combination with different exchange-correlation functionals. In addition, this method delivers a description of the chemical bonding as intuitive as Lewis theory that may bridge the gap between DFT and chemical intuition.

[1] J. P. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)

[2] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)

[3] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)

[4] T. Hahn et. al., J. Chem. Phys., vol- 143, 224104 (2015)

CPP 10.8 Mon 12:15 HL 001

First-principles modeling of mixed-valence compounds from extended Hubbard-corrected functionals — •Matteo Cococcioni and Nicola Marzari — Theory and Simulations of Materials and MARVEL, EPFL, Lausanne, Switzerland

Modeling the electronic properties of mixed valence compounds is central to developing many materials of technological relevance. Unfortunately, most approximate implementations of density functional theory (DFT) fail in capturing the localization of valence electrons on low dispersion states (e.g., of d or f kind) and mis-represent many properties of these systems. Quantitatively predictive first-principles calculations thus require, for these systems, the use of corrective functionals able to improve the description of electronic localization. Using the results of a recent study on materials for cathodes of Li-ion batteries this work shows how an extended Hubbard correction to DFT functionals, including on-site (U) and inter-site (V) interactions (named DFT+U+V) improves considerably on simpler approximations for electronic, magnetic and structural properties and correctly describes localized states even in presence of significant inter-site hybridization. The work also demonstrates that evaluating the effective interaction parameters (U and V) consistently with the electronic and crystal structures, and treating them as material-specific quantities, improves the prediction of thermodynamic quantities and of average voltages. Finally, a novel method to compute these interactions from density-functional perturbation theory is shown to guarantee unprecedented efficiency, accuracy and convergence control.

CPP 10.9 Mon 12:30 HL 001

A Kohn-Sham type construction on a lattice with the exact kinetic energy density — •Iris Theophilou[1], Michael Ruggenthaler[1], Florian Buchholz[1], Florian Eich[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

In this presentation we explore a possible formulation of ground state Density Functional Theory by introducing the kinetic energy density as basic quantity in addition to the density. We presently restrict this formulation to the lattice case, and show that for a few site Hubbard interacting model it is numerically feasible to find an equivalent non-interacting system that yields the same density and kinetic energy density. By finding such a non-interacting system we mean here finding the local/on site potential and the non-local site dependent hopping that will give the target density and kinetic energy density. Our hope is that by including the kinetic energy density we will facilitate the functional construction and also put into grounds already existing approximations based on this quantity.

CPP 10.10 Mon 12:45 HL 001

Small-Polaron Formation in Polymorphs of Ga_2O_3 and TiO_2 — •Sebastian Kokott, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin 14195, Germany

Transparent oxides are key materials for new devices in photovoltaics and electronics. One important factor influencing the behavior of charge carriers in these materials is the interaction with polar phonon modes. We focus on materials with strong electron-phonon coupling, where small polarons are formed. Although, density-functional theory (DFT) is often used for calculating polaron properties, there are two challenges: Sensitivity of the calculated properties to the errors in exchange-correlation treatment, and finite-size effects in supercell calculations. We have developed an approach [1] to address these issues. The polaron properties are obtained using a modified neutral potential-energy surface from DFT [2]. Based on Pekar′s model [3], we correct for the proper elastic long-range behavior of the polaron in a supercell. With this approach, the influence of the crystal structure on the polaron properties is investigated for rutile and anatase TiO_2, and for the monoclinic β– and orthorhombic ε–Ga_2O_3. We find that in rutile TiO_2 only small electron polarons are stable, while only small hole polarons are found in anatase. On the contrary, small hole polarons exist in both Ga_2O_3 polymorphs but have significantly different binding energies.

[1] S. Kokott, arXiv:1710.03722 (2017)
[2] B. Sadigh et al., Phys. Rev. B **92**, 75202 (2015)
[3] S. I. Pekar, Zh. Eksp. Teor. Fiz. **16** 335 (1946)

CPP 11: Responsive and Adaptive Systems

Time: Monday 11:15–13:00 Location: C 230

CPP 11.1 Mon 11:15 C 230

Light-responsive azobenzene star with a flat core — •Markus Koch[1], Marina Saphiannikova[1], Svetlana Santer[2], and Olga Guskova[1] — [1]Institute Theory of Polymers, IPF Dresden, Germany — [2]Institute of Physics and Astronomy, University of Potsdam

This study focuses on comparing physical properties of photoisomers of an azobenzene star with benzene-1,3,5-tricarboxamide core. Three azobenzene arms of the molecule undergo a reversible trans-cis isomerisation upon UV-vis light illumination giving rise to multiple states from the planar all-trans one, via two mixed states to the kinked all-cis isomer. To characterize the light-triggered switching of solvophilicity/solvophobicity of the star, the difference in solvation free energy is calculated for the transfer of an azobenzene star from its gas phase to implicit or explicit solvents. From the analysis of two contributions to the free energy of hydration, the non-polar van der Waals and the electrostatic terms, calculated using soft LJ and Coulomb potentials [1] we conclude that isomerization state largely determines the polarity of the molecule and the solute-solvent electrostatic interactions. This convertible hydrophilicity/hydrophobicity together with re-adjustable occupied volume and the surface area accessible to water, explains the physics of the self-assembly/disassembly of the azobenzene star with a flat core triggered by light.

This work was supported by DFG (Project No GU 1510/3-1 and SA 1657/13-1).

[1] M. Koch et al. J. Phys. Chem. B 2017, 121, 8854.

CPP 11.2 Mon 11:30 C 230

Photomigration in azo-polymer thin films probed by atomistic molecular dynamics simulations — •Marcus Böckmann and Nikos Doltsinis — Institut für Festkörpertheorie, Westfälische Wilhems-Universität, Münster, Germany

Photoresponsive polymers containing azobenzene (AB) as the photochromic unit are well known for allowing photopatterning and the fabrication of surface relief gratings (SRGs) [1,2]. In this contribution, we will report on recent results from our theoretical studies based on multiscale molecular dynamics (MD) simulation techniques [3,4] applied to the phenomenon of light-induced mass transport – also being termed photofluidity [5] – in an active layer slab of poly-disperse-orange-3-metacrylamide (PDO3M) [6].

[1] P. Rochon, E. Batalla, and A. Natansohn, *Appl. Phys. Lett.* **66**, 136 (1995).
[2] N.S. Yadavalli, F. Linde, A. Kopyshev, and S. Santer, *ACS Appl. Mater. Int.* **5**, 7743 (2013).
[3] M. Böckmann, D. Marx, C. Peter, L. Delle Site, K. Kremer, and N. Doltsinis, *Phys. Chem. Chem. Phys.* **10**, 1039 (2011).
[4] M. Böckmann, S. Braun, N. L. Doltsinis, and D. Marx, *J. Chem. Phys.* **139**, 084108 (2013).
[5] P. Karageorgiev, D. Neher, B. Schulz, B. Stiller, U. Pietsch, M. Giersig, and L. Brehmer *Nature Materials* **4**, 699 (2005).
[6] M. Böckmann and N. L. Doltsinis, *J. Chem. Phys.* **145**, 154701 (2016).

CPP 11.3 Mon 11:45 C 230

Smart Air/Water Interfaces with Arylazopyrazol Surfactants and their Role in Responsive Aqueous Foam — •Marco Schnurbus[1], Lucas Stricker[2], Bart Jan Ravoo[2], and Björn Braunschweig[1] — [1]Institute of Physical Chemistry — [2]Organic Chemistry Institute, WWU Münster, 48149 Münster, Germany

A new light-switchable azo-surfactant arylazopyrazol tetraethylen glycol carboxylic acid (AAP-E_4) was used as a building block to functionalize macroscopic foams. AAP-E_4 was studied in the bulk with UV/Vis spectroscopy and at the interface with sum frequency generation as well as tensiometry. Foaming experiments were done with a dynamic foam analyzer in order to study the role of AAP-E_4 surfactants within macroscopic foam. In the bulk, it is possible to switch the AAP-E_4 surfactant reversibly from trans to cis configurations and vice versa using 380 nm UV and 520 nm green light. At the interface, we demonstrate excellent switching ability of AAP-E_4 surfactants. We show that the responsiveness of the interface is strongly influenced by lateral electrostatic interactions. Consequently, the disjoining pressure and thus the foam stability are highly dependent on the bulk pH and the charging state of the interface. For that reason, we have studied both the surface net charge and the surface excess as important parameters that determine foam stability in this system and show that neutral pH conditions lead to the best compromise between switching ability, surface excess and surface charging. Measurements on the foam stability demonstrated that foams under illumination with green light are more stable compared to foams illuminated with UV light.

CPP 11.4 Mon 12:00 C 230

Spiropyran ring opening reactions to measure forces on the molecular scale — •Oliver Brügner and Michael Walter — FIT Freiburger Zentrum für interaktive Werkstoffe und bioinspirierte Technologien, Universität Freiburg

Spiropyrans are mechanochromatic molecules which change color under the influence of force. These molecules can be integrated into polymers. By stretching the polymer, mechanical forces are transferred to spiropyran and lead to a ring opening reaction. Thereby the colorless spiropyran transforms into the colored merocyanine form. This reaction is reversible and the back reaction is already induced by thermodynamic excitations at room temperature [Kem]. Therefore spiropyran can be used as a molecular switch and belongs to the group of interactive materials.

In order to understand the molecular insides needed for using spiropyran as the responsive material in polymeric force sensors in the future, we investigated the energetics of spiropyran based on density functional theory and added entropic effects of the polymer. The model used is a combination of a relatively simple description of the polymer combined with an accurate description of the spiropyran ring opening reaction. We determine the dependence of the force on the polymer stretching length and find a very good agreement with experimental results from single molecule AFM experiments.

[Kem] Fabian Kempe, Oliver Brügner, Hannah Buchheit, Sarah N. Momm, Felix Riehle, Sophie Hameury, Michael Walter, and Michael Sommer, Angew. Chem. Int. Ed. 56 (2017) 1-5

CPP 11.5 Mon 12:15 C 230

Thermo-Responsive Foams from Aqueous Hydroxylpropyl Cellulose Solutions — •Eric Weissenborn and Björn Braunschweig — Institute of Physical Chemistry, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany

We have studied the ability of hydroxypropyl cellulose (HPC) with a molecular weight of 1 MDa to switch macroscopic foam reversibly from stable to unstable conditions. At 25°C room temperature, foams from 0.5 μM HPC are extremely stable with lifetimes of several hours. However, we can dramatically reduce the foam stability by increasing the temperature to 50°C which is well above the lower critical solution temperature (LCST) of 45°C. In order to clarify the underlying mechanism, we investigated the adsorption of HPC at the air/water interface by recording dynamic surface tensions using the pendant drop method. In addition, UV-VIS spectroscopy and dynamic light scattering indicate the formation of aggregates in the bulk for temperatures above the LCST. Bulk rheology of HPC dilutions shows that at these temperatures, the solutions viscosity is substantially decreased and as a consequence the foam drainage is increased. The latter decreases the foam stability, because foam drainage is one of the major destabilization mechanisms in this system. A fast reduction of temperature from 50°C to 25°C solubilizes the polymer reversibly and leads to a stabilization of the foam back to its initial stability.

CPP 11.6 Mon 12:30 C 230

Density and temperature dependence on supramolecular polymer morphology of polyethylene and polybutylene glycols with hydrogen bonding ends — •Eunsang Lee and Wolfgang Paul — Institut für Physik, Martin-Luther Universität Halle-Wittenberg, Halle, Germany

Rheological properties of supramolecular polymers depend on their structure including the size, the number, and the topology of aggregates. A polymer with a hydrogen-bonding motif at both ends is one widely used precursor to build the supramolecular polymers. In this work we investigate structures of supramolecular polyethylene glycol and polybutylene glycols with associating ends in wide range of temperature and density using a coarse-grained (CG) model via stochastic approximation Monte Carlo method. Our CG force field is constructed by Boltzmann inversion of the probability distributions of all-atom polymer conformations. This work especially focuses on the transition from ring- to chain-dominated phases since the ring contaminant in a ring-linear blend melt is known to significantly influence its rheology. The phase diagram in a density-temperature space displays two continuous transition lines. One is the transition from ring- to chain-dominated phase with a coexistence between two phases at the transition temperature and the other is the transition from chain-dominated to free chain phase. For supramolecular polymers at melt-like density it turns out that chain aggregates dominate over rings at room temperature.

CPP 11.7 Mon 12:45 C 230

Single dendronized macromolecules as force probes for 2D interaction forces — •Mohammad Fardin Gholami[1], Jose D. Cojal Gonzalez[1], Simone DellElce[1], Vitalij Scenev[1], Nikolai Severin[1], Baozhong Zhang[2], A. Dieter Schlüter[2], and Jürgen P. Rabe[1] — [1]Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin — [2]Department of Materials, Institute of Polymers, ETH Zürich

Graphene can replicate the topography of a substrate with a precision down to single macromolecules [1]. Here we use this capability and investigate the deformation of the macromolecules under graphene based 2D materials.We sandwiched cylindrically shaped dendronized polymers (denpols) between mica and graphene oxides (GO), reduced graphene oxides (rGO), and graphenes. The cross section of the denpols can be systematically varied through the dendron generation. The height of the molecular imprints in GO agrees with the height of those on bare mica while the height of molecular imprints in graphenes are smaller than the height of uncovered molecules, with the difference growing with the dendron generation. The heights of molecular imprints in rGO are in between those for graphene and GO. We attribute this to a larger interaction between those sheets and the mica, effectively squeezing the molecules as observed also in steered MD simulations. The combination of these experimental and theoretical results imply that it is possible to measure the interaction forces between 2D sheets and substrates by using the macromolecules as force sensors.

[1] N. Severin, *et al. Nano Lett.* 11 (2011) 2436.

CPP 12: Focus: Molecularly Functionalized Low-Dimensional Systems II - organized by Antonio Setaro, Carola Meyer, Aravind Vijayaraghvan and Matteo Mannini

See part I of the session for a synopsis.

Time: Monday 15:00–17:30 Location: C 130

Topical Talk CPP 12.1 Mon 15:00 C 130

Magnetoresistance in Single-Radical Molecular Junctions — •Elke Scheer — Department of Physics, University of Konstanz, 78457 Konstanz

We study the charge transport properties of single radical molecule junctions formed by a break junction technique at 4.2 K in magnetic field B. In this study, stable and neutral radical molecules based on an oligo(p-phenylene ethynylene) (OPE) backbone with a radical attAched to its side (TEMPO-OPE) are contacted with freestanding and tunable gold (Au) electrodes. In perpendicular field we observe large positive magnetoresistance (MR) up to 287 % at 4T [1]. The average MR amplitude is one order of magnitude larger than that of the analogous non-radical OPE molecule. In parallel field a step-like negative MR occurs with the same amplitude on field scales of 2-3 T. The analysis of the MR, of current-voltage characteristics and of inelastic electron tunneling spectra reveal an effective reduction of the electronic coupling between the current-carrying frontier orbital and the metal electrodes with increasing B. Our findings thus provide a new physical approach for tuning the charge transport through radical molecules. [1] R. Hayakawa et al. Nano Lett. 16, 4960 (2016).

CPP 12.2 Mon 15:30 C 130

UHV deposition of pyrene on metal surfaces — •Sebastian Schleicher[1], Bogdana Borca[3], Jeff Rawson[2], Frank Matthes[1], Daniel E. Bürgler[1], Paul Kögerler[2], and Claus M. Schneider[1] — [1]Peter Grünberg Institut (PGI-6), Forschingszentrum Jülich — [2]Institute of Inorganic Chemistry, RWTH Aachen Universität — [3]National Institute of Materials Physics, Bucharest, Romania

Interfacial properties of organic adsorbates featuring aromatic π-orbitals on metal surfaces play an important role for organic electronics and spintronics. The deposition of single pyrene molecules with a size between ultimately small benzene and extended graphene on clean and reactive surfaces is challenging, since pyrene is a solid with a high vapor pressure. Hence, it cannot be evaporated from a Knudsen cell, nor dosed from the gas phase. Here, we present a sublimation procedure under UHV and image pyrene molecules on in-situ cleaned Au(111) and Fe/W(110) substrates by means of low temperature scanning tunneling microscopy (LT-STM) at 77 K. For the Au(111) surface, the molecule-surface interaction is weak such that the Au(111) herringbone reconstruction is not lifted and visible through the ordered molecular layer. Pyrene desorption self-limits growth to a monolayer due to the weak intermolecular bonding. The molecular arrangement of adsorbed pyrene on stronger interacting Fe films on W(110) sensitively depends on Fe thickness. Irregular configurations occur on the first Fe layer, while self-assembled ordered arrays form on the second, third and fourth Fe layer.

CPP 12.3 Mon 15:45 C 130

Spin-Dependent Electron Transmission Model for Chiral Molecules in Solid-State Nanodevices — •Xu Yang — Zernike Institute for Advanced Materials, University of Groningen, Groningen, the Netherlands

Various experiments have indicated that electron-transfer in several chiral molecules is spin-dependent, a phenomenon known as the Chiral Induced Spin Selectivity effect. This holds promise for realizing spintronic nanodevices that do not contain ferromagnetic materials. However, due to the lack of theoretical understanding, it is not always clear to what extent the chiral molecules contribute to the spin-dependent signals. We aim to develop a spin-dependent electron transmission model that can quantitatively evaluate the role of chiral molecules in two-terminal, three-terminal and four-terminal transport measurements. As starting point, we use the universal symmetry of electrical conduction to explain the necessity of spin-flip electron reflection at chiral molecules. Based on this model, we propose new types of graphene- or carbon nanotube- based multi-terminal transport measurements that can separate the CISS effect from other spin-dependent signals. Our modeling provides a fundamental insight and an effective toolbox for understanding low-dimensional solid-state spintronic devices functionalized with chiral molecules.

CPP 12.4 Mon 16:00 C 130

Electrical Characterization of Bis(terpyridine)ruthenium-Complex Functionalized Au-Nanoparticles in Heterometallic Nanoelectrode Gaps — •Max Mennicken[1], Sophia Knecht[2], Corinna Kaulen[2], Ulrich Simon[2], and Silvia Karthäuser[1] — [1]Peter Grünberg Institut (PGI-7), Forschungszentrum Jülich GmbH, Germany — [2]Institut für Anorganische Chemie (IAC), RWTH Aachen University, Germany

Following the concept of integrating molecular electronic devices into traditional CMOS circuitry, molecularly functionalized metal nanoparticles (NP) are employed. Especially complexes of ruthenium with chelating terpyridine ligands exhibit interesting properties. They can act as a switch of constant length, based on a redox mechanism, addressed by electrical or optical pulses. The application of 1,4-bis(2,2':6',2"-terpyridin-4'-yl)benzol (BTP) ligands as a linear linking moiety allows the formation of Ru-BTP diads, triads or even longer molecular wires. Here, we use 15 nm Au-NP functionalized with 4'-(4-mercaptophenyl)-2,2':6'2"-terpyridin (MPTP) and the corresponding (MPTP)$_2$-ruthenium complex. We immobilized such Au-NP in between heterometallic nanoelectrode gaps consisting of AuPd and Pt. The resulting devices are characterized by SEM and transport measurements which are compared to estimations of the conductance through the respective molecules. Furthermore, the principle of growth of Ru-BTP based molecular wires is investigated by XPS measurements.

CPP 12.5 Mon 16:15 C 130

Impact of chemical treatment of diamond thin films on neuron growth — Barbora Jakubcová[1], Jana Turňová[1], Václav Petrák[1], Pavel Hubík[2], Andrew Taylor[2], and •Vladimíra Petráková[1,3] — [1]Czech Technical University in Prague, Faculty of Biomedical Engineering, Kladno, Czech Republic — [2]Czech Academy of Sciences, Institute of Physics, Prague, Czech Republic — [3]Free University Berlin, Institute of Experimental Physics, Berlin, Germany

This work compares the impact of molecular functionalization and selected material properties of diamond thin films on the growth of neurons. The ability to form an efficient interface between material and neural cells is a crucial aspect of the construction of neuroelectrodes. Diamond thin films offer material characteristics that could greatly improve the performance of neuroelectrodes. The advantage of diamond is a large variety of material and surface properties. Such a variety of material characteristics can lead to various cellular responses. Here we compare growth and development of primary neural cells on diamond thin films of various morphology, conductivity, and doping with their treatment using several types of molecules commonly used to enhance adhesion and cell growth. We found that the variation of material properties of nanocrystalline diamond film does not have a major influence on the neuron growth but it can be to, some extent, influenced by the type of molecular coating, selection of polymer and its molecular weight. Our findings emphasize the importance of the correct molecular treatment over structural or morphological properties of diamond thin films as a material used to form an interface with primary neurons.

15 min. break

CPP 12.6 Mon 16:45 C 130

Nanowire field-effect transistor structures for the detection of cardiac biomarkers: troponin and C-reactive protein — Yurii Kutovyi, Ihor Zadorozhnyi, Volodymyr Handziuk, Hanna Hlukhova, Nazarii Boichuk, and •Svetlana Vitusevich — Bioelectronics (ICS-8), Forschungszentrum Juelich, 52425 Juelich, Germany

Today high-speed operation is one of the key factors in the development of biosensors. Cardiac disease is one of the most critical diseases, requiring medical treatment within the first two hours of acute myocardial infarction (AMI). Cardiac troponin (cTn) remains the gold standard in AMI diagnosis. cTn is released from the cardiac cell and its concentration typically increases after the onset of AMI. At the same time, C-reactive protein (CRP) can be used as a predictive biomarker to indicate the likelihood of AMI in the near future. In this presentation, we will discuss the design and fabrication of silicon nanowire field-effect transistor structures using CMOS-compatible technology as well as the results we obtained upon the detection of both proteins. We demonstrate that along with the threshold voltage shift measured as a function of charged molecule binding events, a number of new parameters due to single-trap phenomena can be used as the detection signal. Together with a gate coupling effect, the utilization of new parameters allows more sensitive monitoring of troponin and CRP behavior in addition to the realization of real-time compact devices for point-of-care applications. Authors gratefully acknowledge the Innovation Award RWTH transparent 2016.

CPP 12.7 Mon 17:00 C 130

Ultrasensitive and selective detection of biomarkers with bio-functionalized graphene field effect transistors — •David Kaiser[1], Nikolaus Meyerbroeker[2], Werner Purschke[3], Andreas Winter[1], Christof Neumann[1], Thomas Weimann[4], Albert Schnieders[2], Axel Vater[3], and Andrey Turchanin[1] — [1]Institute for Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]CNM Technologies GmbH, 33607 Bielefeld, Germany — [3]APTARION biotech AG, 10589 Berlin, Germany — [4]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

Due to the unique properties of graphene, graphene-based field effect transistors (GrFETs) are promising electronic devices for sensing of biological molecules. In this contribution, we present a concept of novel hybrid BioGrFETs for selective and ultrasensitive detection of biomarkers based on graphene functionalized non-covalently with L-aptamers via a molecular carbon nanomembrane (CNM). We demonstrate that the engineered BioGrFETs have up to 3 orders of magnitude dynamic range and reach a sensitivity limit down to 1 pM for selected biomarkers. We characterize the subsequent fabrication steps on the nanoscale by surface science and biochemical techniques and describe the BioGrFETs transfer characteristics by an electrochemical model of the heterostructure interface.

CPP 12.8 Mon 17:15 C 130

Proton Transport Through 2D Membranes — •Yun An[1], Agnieszka Kuc[1], Petko Petkov[2], and Thomas Heine[1] — [1]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Leipzig, Germany — [2]Faculty of Chemistry and Pharmacy, University of Sofia, 1164 Sofia, 1 James Bourchier Blvd., Bulgaria

Conventional membranes have been used for sieving atomic and molecular species, however, they have no subatomic selectivity. Recently, two dimensional (2D) crystals, such as graphene and hexagonal boron nitride (hBN), have been shown to be good candidates for hydrogen isotope sieving. Nevertheless, the mechanism of such a process has not been reported so far. Therefore, to understand the proton transport through 2D membranes is of great importance. Aiming at this, we have studied theoretically what happens with protons when introduced between 2D layers. Density functional theory (DFT) together with well-tempered metadynamics simulations was employed to study dynamics of proton transfer in between the layers. Our studies reveal that lattice vibrations are crucial for understanding the phonon calculations. While they can be well described using Born-Oppenheimer DFT based metadynamics simulations, static transition state calculations at the same level of theory lead to very high barriers that are unsuitable to describe the experimental observations.

CPP 13: Organic Electronics and Photovoltaics - Hybrid and Organic Layer Systems

Time: Monday 15:00–16:30 Location: C 243

CPP 13.1 Mon 15:00 C 243

Electrical characterization of hybrid n-GaN/p-PEDOT structures for optoelectronic applications — •Linus Krieg[1], Daniel Splith[2], Zhipeng Zhang[2], Holger von Wenckstern[2], Marius Grundmann[2], Florian Meierhofer[1], Xiaoxue Wang[3], Karen Gleason[3], and Tobias Voss[1] — [1]Institute of Semiconductor Technology and Laboratory for Emerging Nanometrology, Braunschweig University of Technology, 38092 Braunschweig — [2]Felix-Bloch-Institut für Festkörperphysik, Halbleiterphysik, Linnéstr. 5, 04103 Leipzig — [3]Department of Chemical Engineering, Massachusetts Institute of Technology, 02139 Cambridge

Hybrid structures consisting of both inorganic and organic conductive layers are promising for the development of inexpensive, versatile and tailored electronic and optoelectronic devices such as sensors or light emitting diodes (LEDs). We study the fabrication of planar n-GaN/p-PEDOT heterostructures. The p-polymer is grown via oxidative chemical vapor deposition (oCVD), a dry deposition approach that allows for controllable polymer deposition out of the gas phase while achieving conformal coverage of the substrate with a thickness control of the deposited polymer layer in the nanometer range. We analyze the temperature-dependent current-voltage characteristics of the hybrid GaN/PEDOT-structures to study the electronic properties of the hybrid interface. The results show a pronounced diode characteristic of the hybrid device and allow us to deduce the relevant conduction mechanisms. We deduce the saturation current of the device and develop a model of the band lineup hybrid n-inorganic/p-organic interface.

CPP 13.2 Mon 15:15 C 243

Bias dependency of hybrid charge transfer emission at planar ZnO/small molecule interfaces — •Stefan Zeiske[1], Ulrich Hörmann[1], Fortunato Piersimoni[1], Lukas Hoffmann[2], Thomas Riedl[2], Denis Andrienko[3], and Dieter Neher[1] — [1]Universität Potsdam, Germany — [2]Bergische Universität Wuppertal, Germany — [3]MPI Mainz, Germany

Recent studies propose that the electroluminescence from hybrid charge transfer excitons (HCTX) depends not only on the interfacial energy gap but also on the applied bias. The models to explain these observation base either on filling of trap states, or on the assumption of delocalized HCT state confined in a triangular quantum well created by the electric field. Here, we investigate the origin of the bias dependent HCTX emission at planar interfaces between the ZnO and different small molecules. We find a nearly linear dependency of the EL peak position on the applied electric field. The independency of the slope on the organic layer thickness confirms that the shift is caused by a field and reminds of the linear Stark effect. Simple 1D quantum mechanical models confirm this interpretation and predict a moderate hole delocalization in the organic of the order of the typical size of a small molecule. Electrostatic treatment of the interaction of the charged molecule with its image potential, however, reveals that the observed field dependence is considerably influenced by the polarizability of the organic cation. As a direct consequence the field-induced shift of the EL peak is expected to be strongly dependent on the molecular orientation at the hybrid interface.

CPP 13.3 Mon 15:30 C 243

Energetics of polar organic metal-insulator-semiconductor diodes probed by different techniques — •Alexander Hofmann[1], Simon Züfle[2], Stéphane Altazin[2], Kohei Shimizu[3], Beat Ruhstaller[2], Hisao Ishii[3], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Institute of Computational Physics, ZHAW, 8401 Winterthur, Switzerland — [3]Center for Frontier Science, Chiba University, Chiba, 263-8522 Japan

The strong dipole moment of polar organic materials like tris-(8-hydroxyquinolate) aluminum (Alq$_3$), if not oriented perfectly anisotropic, will lead to the buildup of a giant surface potential (GSP) of the organic film. As we have shown previously [1], it is possible to apply the CELIV (Charge Extraction by Linearly Increasing Voltage) method on polar diodes to determine the charge transport activation energy. Combined with impedance spectroscopy, this technique can be used to measure the injection barrier of the underlying metal-semiconductor interface [2]. In this contribution, we show the practical performance of this method compared to ultra violet photoelectron spectroscopy as an established method of determining injection barriers. We have applied the technique to the prototypical polar organic system *N*,*N*'-Di(1-naphthyl)-*N*,*N*'-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB) and Alq$_3$ in different dilutions and show the dependence of the determined barrier on the dilution ratio.

[1] Journal of Applied Physics **121**, 175501 (2017) [2] Journal of Applied Physics **122**, 115502 (2017)

CPP 13.4 Mon 15:45 C 243

Theoretical determination of the ionization potential and the electron affinity of organic semiconductors — •Susumu Yanagisawa — University of the Ryukyus

Ionization potential (IP) and electron affinity (EA) of organic semiconductors are important quantities, which are relevant to barriers for injection of charge (hole or electron). The electrostatic and electronic polarization contributions to the polarization energies for the injected charges in pentacene polymorphs were investigated with first-principles calculations. The former contribution was estimated by employing periodic slabs of the surfaces at the semi-local density functional level of theory. On the other hand, the latter was treated for the bulk systems at the many-body perturbation theory within the GW approximation. It was found that while the electronic polarization induced narrowing of the energy gap in the single crystal and the thin film phases, the electrostatic effect shifted up or down the frontier energy levels such as the highest-occupied molecular orbital- (HOMO) and the lowest-unoccupied molecular orbital-derived (LUMO) levels relative to the vacuum level, sensitively to the molecular orientation at the surface. The role of the electrostatic interaction such as the charge-permanent quadrupole interaction dominating IP and EA of the materials is discussed.

CPP 13.5 Mon 16:00 C 243

Hot electrons and hot spins at metal-organic interfaces — •Thorsten Arnold[1], Ainhoa Atxabal[2], Subir Parui[2], Luis E. Hueso[2], and Frank Ortmann[1] — [1]Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany — [2]CIC nanoGUNE, 20018 Donostia-San Sebastian, Basque Country, Spain

Metal-organic barriers between the metal Fermi energy and the molecular levels of the organic semiconductor play a fundamental role in the performance of organic electronic devices. In order to measure these barriers, recently, a hot-electron transistor device has been developed [1]. We propose a theoretical model [2], which describes all the transport effects of the hot electrons for the first time. The model is able to reproduce the experimental results with excellent accuracy.

The model is extended to predict the transport characteristics of spin-polarized hot electrons in these devices. We find a spatial variation of the spin diffusion length, which scales inversely proportional to the variation of the electron density. The spin current can be increased by increasing the hot electron energy and by decreasing the image charge barrier without changing the spin diffusion length. We also provide unprecedented insight into the effects of disorder at the metal-organic interface. Finally, we establish conditions when pure spin currents appear, where majority and minority spin carriers propagate in opposite directions.

[1] A. Atxabal et al., Adv. Mater. 29, 1606901 (2017).

[2] T. Arnold et al., Adv. Funct. Mater. (to be published).

CPP 13.6 Mon 16:15 C 243

Exciting Strong Fano Resonances by Stacking Plasmonic Nanostructures — •Ye Yu[1], Ziwei Zhou[2], Tobias A. F. König[1,3], and Andreas Fery[1,3,4] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Straße 6, 01069, Dresden, Germany — [2]State Key Laboratory of Supramolecular Structure and Materials, Jilin University, Changchun, China — [3]Cluster of Excellence Centre for Advancing Electronics Dresden (cfaed), Technische Universitat Dresden, 01062 Dresden, Germany — [4]Department of Physical Chemistry of Polymeric Materials, Technische Universitat Dresden, Hohe Str. 6, 01069 Dresden, Germany

Small gaps at nanometer-scale enabled noble metals to be perfect research of interest in the field of plasmonic sensing devices, optical antennas, and nanolasing systems. Due to the ultra-small gap formed in between two metallic components, the coupling effect is usually enormous and hence extreme nanoscale confinement and enhancement of the near electric field intensity. Despite the huge potential in these nanogap devices, challenges still remain in manufacturing the advanced devices with high throughput and reproducibility. Here we propose to fabricate nanogap structures with a combination of bottom-up assembly and top-down patterning strategy in the mean of lower cost and higher throughput. We were able to fabricate nanogap structures of high quality and also over large area. The optical properties proven to be of high electric field enhancement with the possibility of exciting Fano resonances due to the plasmonic hybridization between two metallic parts forming the nanogaps.

CPP 14: Interfaces and Thin Films I

Time: Monday 15:00–17:45 Location: C 264

CPP 14.1 Mon 15:00 C 264

Permittivity at Liquid-Liquid Interfaces: An Iterative Reaction Field Approach — •David Egger, Karsten Reuter, and Christoph Scheurer — TU München

Realistic models for catalytic reactions at liquid-liquid interfaces require a profound knowledge of the electrostatic properties in the vicinity of the solvated catalytic complex. For polar fluids like water, these properties as described by the static dielectric constant, ε, can be related to thermal equilibrium fluctuations of the polarization at zero field. The Kirkwood-Fröhlich (KF) approach usually applied in the derivation of such formulas faces two major difficulties: First, correlated polarization fluctuations are long-range and subject to slow convergence, making KF expensive in simulations. Second, the difficulty of the electrostatic boundary value problem one needs to solve in a KF ansatz increases with the systems' complexity. In this contribution, we present a possible alternative procedure, following the reaction field approach described by Neumann for cubic and spherical sample shapes [1]. Exploiting the constant reaction field of oblate spheroidal dielectric bodies immersed in continuum dielectrics, we present an iterative method to calculate a spatially resolved ε from cavities of different shape and volume, avoiding difficulties with geometry-induced boundary conditions in the electrostatic description. Gaussian error regression is further applied to drive down statistical errors, exploiting the presupposed continuitiy of the dielectric tensor field. Results are discussed for water bulk and water-dichloroethane interfacial systems.

[1] M. Neumann, Mol. Phys. 50, 841 (1983).

CPP 14.2 Mon 15:15 C 264

On the Origins of the Charging of Water at the Air-Water Interface — •Emiliano Poli[1], Ali Hassanali[1], and Himanshu Mishra[2] — [1]The Abdus Salam International Centre for Theoretical Physics (ictp), Trieste, Italy — [2]King Abdullah University of Science and Technology Thuwal, Saudi Arabia

Aqueous interfaces are ubiquitous in nature and technological applications. Numerous physical, chemical and engineering processes occur at interfaces involving water and hydrophobic surfaces. Despite long study, many issues still remain controversial regarding the properties of water at hydrophobic interfaces. One particular interface in this regard that has received a lot of attention is the air-water interface. In particular, the origin of the surface charge of water, remains elusive.

In this work we investigate the electronic properties of the air-water interface using state-of-the-art linear scaling DFT methods allowing us to model systems consisting of over thousands of atoms. We examine how the dipole and quadrupole moments of water change near the interface as well as how charge transfer between layers is rooted in topological properties of the water network such as coordination defects and water wires. The role of both classical electrostatics and quantum mechanical effects like charge transfer and exchange, are examined with respect to the affinity of protons and hydroxide ions for the surface of water.

Finally these results are discussed within the broader framework of water near hydrophobic interfaces such as oil, proteins and hydrophobic polymers.

CPP 14.3 Mon 15:30 C 264

Monitoring the Swelling Behavior of PEDOT:PSS Electrodes under High Humidity Conditions — •Lorenz Biessmann[1], Lucas Philipp Kreuzer[1], Tobias Widmann[1], Nuri Hohn[1], Jean-François Moulin[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]HZG at MLZ, 85748 Garching

One main advantage of organic electronics is the enabling of building flexible electronic devices. The polymer mixture poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) offers good electrical conductivity, transparency and inherent flexibility, which makes it to a promising alternative to rigid and brittle transparent electrodes like indium tin oxide (ITO). By different treatment methods it is possible to adjust the conductivity and work function of PEDOT:PSS to its desired requirements. The hygroscopic behavior of the PSS component yields a high potential for water uptake of the PEDOT:PSS. This is known to have a negative influence on its electronic conductivity. Furthermore, an increasing film thickness due to water uptake may lead to mechanical stress on the other functional layers in the organic device. Hence, we investigate the PEDOT:PSS thin films regarding their swelling behavior under high humidity conditions, using in-situ time of flight neutron reflectivity (TOF-NR) measurements. Two commonly used PEDOT:PSS treatments are compared to pristine PEDOT:PSS. We observe a strong dependence of water uptake and thickness evolution on the type of PEDOT:PSS treatment.

CPP 14.4 Mon 15:45 C 264

Controlling Adhesion and Friction on Cyclodextrin Assemblies — •Johanna Blass[1,2], Marcel Albrecht[3], Gerhard Wenz[3], and Roland Bennewitz[1,2] — [1]INM - Leibniz-Institute for New Materials, Campus D2 2, Saarland University, 66123 Saarbrücken, Germany — [2]Physics Department, Saarland University, Campus D2 2, Saarland University, 66123 Saarbrücken, Germany — [3]Organic Macromolecular Chemistry, Campus C4 2, Saarland University, 66123 Saarbrücken, Germany

Controlling and understanding adhesive interactions on the molecular scale is one of the main challenges in the field of nanotechnology. We developed a new surface functionalization based on assemblies of cyclodextrin molecules to control adhesive forces and study the molecular mechanisms underlying dynamic effects of adhesion and friction. The dynamics of the molecular system were studied with respect to multivalency effects, single bond kinetics and flexibility of the attachment. By varying the compliance of the surface attachment, the relation between adhesion and friction and their dynamic rupture characteristics can be tuned. The rupture force of single bonds in thermodynamic equilibrium increases proportional to the square root of the force probe stiffness and is not determined by the stiffness of the molecular linker. The applicability of the surface functionalization was demonstrated when attaching cyclodextrin molecules onto stiff polymers to bridge the surface roughness of real contacts. Active control of adhesion and friction was achieved using photosensitive connector molecules which are sensitive to external light stimuli.

CPP 14.5 Mon 16:00 C 264

Multivalent-Ion-Activated Protein Adsorption Reflecting Bulk Reentrant Behavior — •Madeleine Fries[1], Daniel Stopper[2], Michal K. Braun[1], Alexander Hinderhofer[1], Fajun Zhang[1], Robert M. J. Jacobs[3], Maximilian W. A. Skoda[4], Hendrik Hansen-Goos[2], Roland Roth[2], and Frank Schreiber[1] — [1]Institute for Applied Physics, University of Tübingen — [2]Institute for Theoretical Physics, University of Tübingen — [3]Department for Chemistry, Chemistry Research Laboratory, University of Oxford, UK — [4]Rutherford-Appleton Laboratory, ISIS Facility, Didcot, UK

Protein adsorption at the solid-liquid interface is an important phenomenon that often can be observed as a first step in biological processes. Despite its inherent importance, still relatively little is known about the underlying microscopic mechanisms. Here, using multivalent ions, we demonstrate the control of the interactions and the corresponding adsorption of net-negatively charged proteins (BSA) at an interface (SiO_2) by ellipsometry. We show that the reentrant condensation observed within the rich *bulk* [1] phase behavior of the system featuring a nonmonotonic dependence of the second virial coefficient on salt concentration c_s is reflected in an intriguing way in the protein adsorption $d(c_s)$ at the *interface*. Our findings are successfully described and understood by a model of ion-activated patchy interactions within the framework of classical density functional theory. In addition to the general challenge of connecting bulk and interface behavior, our work has implications for, *inter alia*, nucleation at interfaces [2].

[1] Fries et al, PRL (2017); [2] Zhang et al, PRL (2008).

CPP 14.6 Mon 16:15 C 264

Specific Ion Effects of Nd^{3+} on the Structure and the Charging State of β-Lactoglobulin Adsorption Layers — Manuela Richert and •Björn Braunschweig — Institute of Physical Chemistry, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany

The influence of Nd^{3+} cations on β-Lactoglobulin (BLG) at air/water interfaces was investigated as a function of NdCl$_3$ concentration at a constant protein concentration of 15 μM. In addition, we studied the proteins' bulk charging state with ζ-potential measurements and observe a complete reversal of the ζ-potential from -40 to +25 mV at low and high c(NdCl$_3$), respectively. The zero net charging in the bulk is observed between 25 and 50 μM NdCl$_3$, which is linked to a low colloidal stability. At the air/water interface, vibrational sum-frequency generation (SFG) shows a minimum in intensity of O-H stretching bands and a 180° phase change of the latter bands. We attribute these observations to a change in the net orientation of interfacial water molecules. The extreme charge screening of Nd^{3+} ions leads to a reduction of electrostatic repulsive forces and thus to a higher surface excess of BLG. As a result, the equilibrium surface tension decreases from 57 to 50 mN/m when the NdCl$_3$ concentration is increased to 200 μM. Foams show substantial changes in mean bubble size, stability and foamability as a function of NdCl$_3$ concentration. We relate these observations to changes in electrostatic disjoining pressure at low and intermediate c(NdCl$_3$) until interfacial BLG aggregates lead to non-DLVO stabilization of the foams.

15 min. break

CPP 14.7 Mon 16:45 C 264

Electronically coupled two-dimensional assembly of Cu2-xS nanocrystals for selective vapor sensing applications — •Sonam Maiti[1,2], Santanu Maiti[2], Yvonne Joseph[3], Andreas Wolf[4], Dirk Dorfs[4], Frank Schreiber[2], and Marcus Scheele[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen, Tübingen, Germany — [2]Institute of Applied Physics, University of Tuebingen, Tübingen, Germany — [3]TU Bergakademie Freiberg, Freiberg, Germany — [4]Leibniz Universität Hannover, Hannover, Germany

The fabrication of two dimensional (2D) ordered nanocrystal (NC) superlattice films with unique physical properties has remained a challenge for years [1,2]. Here, we demonstrate a novel method to prepare electronically coupled, monolayered films of Cu2-xS NCs with the organic semiconductor molecule TACuPh, which exhibits fascinating charge carrier transport and optical properties. A systematic temperature dependence of the conductivity of the film is studied over a wide range of temperatures. The results indicate that charge carrier transport is governed by 2D variable range hopping (VRH) in the temperature range (280-30K) and changes from Mott VRH to Efros-Shklovskii VRH below 60 K. The high conductivity is attributed to better interparticle coupling by virtue of TACuPh, which is also evident from GISAXS. Finally, the films show good sensing performance towards 4-methyl-2-pentanone and toluene vapors at 0% relative humidity [3]. [1] X. Huang et al. Adv. Mater. 2014, 26, 2185. [2] M. Scheele et al. PCCP, 2005, 17, 97. [3] Y. Joseph et al. Sensor Actuat B, 2004, 98.

CPP 14.8 Mon 17:00 C 264

Silicon surface functionalization towards biosensing via free standing Si-OH bonds on a non-oxidized surface — •Jessica Hänisch[1], Karsten Hinrichs[2], and Jörg Rappich[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Kekuléstraße 5, 12489 Berlin (Germany) — [2]Leibniz-Institut für Analytische Wissenschaften - ISAS - e. V., ISAS-Berlin, Schwarzschildstraße 8, 12489 Berlin, Germany

Silicon (Si) is widely used as a substrate material for the fabrication of biosensor devices.[1] In the most cases, the starting point of the surface functionalization are the surface hydroxyl groups present on the native oxide layer of the Si. The hydroxyl groups can be easily coupled with a huge variety of different silane molecules, depending on the desired functionalities. However, the present oxide layer between the surface functionalization and the bulk Si has some disadvantages like a high defect density and a lower transconductance.[2][3][4] To overcome these downsides, we developed a synthetic pathway, with which single standing and highly stable hydroxyl groups directly bound to the Si surface can be obtained, which has not been achieved before. The hydroxyl groups were further functionalized to obtain a surface ready for immobilization reactions. [1] N.S.K. Gunda, M. Singh, L. Norman, K. Kaur, S.K. Mitra, Appl. Surf. Sci. 2014, 305, 522. [2] H. Haick, P. T. Hurley, A. I. Hochbaum, P. Yang, N. S. Lewis, J. Am. Chem. Soc. 2006, 128, 8990. [3] Y. Cui, Z. Zhong, D. Wang, W. U. Wang, C. M. Lieber, Nano Lett. 2003, 3, 149. [4] O. Assad, H. Haick, 2008 IEEE International Symposium on Industrial Electronics, 2040.

CPP 14.9 Mon 17:15 C 264

Unexpected behavior of thin PVME/PS blend films investigated by specific heat spectroscopy — •Paulina Szymoniak, Sherif Madkour, and Andreas Schönhals — BAM Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin (Germany)

The structure and molecular dynamics of thin polymer films are of topical interest of soft matter-physics. Commonly, spatial structural heterogeneities of 1D confined thin films (surface, bulk-like and adsorbed layer), are expected to alter the glassy dynamics, compared to the bulk. Here, Specific Heat Spectroscopy (SHS) was used to investigate the glassy dynamics of thin films of an asymmetric miscible PVME/PS 25/75 wt% blend. SHS measurements showed a non-monotonous thickness dependence of the dynamic Tg, on the contrary to the previously investigated PVME/PS 50/50 wt% [1]. For PVME/PS 25/75 wt% thin films ($>$ 30 nm), due to the presence of PVME-rich adsorbed and surface layers, the bulk-like layer experienced a thickness dependent increase of PS concentration. This led to a systematic increase of dynamic Tg. Further decrease of the film thickness ($<$ 30 nm) resulted in a decrease of dynamic Tg, ascribed to the influence of the surface layer, which has a high molecular mobility. This is the first study, which shows deviations of dynamic Tg of thin films, compared to the bulk, resulting from the counterbalance of the influence of the surface and adsorbed layer [2,3]. [1] Yin, H. et al. Macromolecules 2015, 48, 4936. [2] Madkour, S. et al. J. Chem. Phys. 2017, 146, 203321. [3] Madkour, S. et al. ACS Macro Lett. 2017, 6, 1156.

CPP 14.10 Mon 17:30 C 264

Preparation and Characterization of Pentacene Thin Films on SiC Graphene — •Martin Hodas[1], Peter Siffalovic[2], Giuliano Duva[1], Berthold Reisz[1], Michal Bodik[2], Peter Nadazdy[2], Alexander Hinderhofer[1], Alexander Gerlach[1], Eva Majkova[2], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Slovak Academy of Sciences, Slovakia

We report on the results of thin pentacene deposition on epitaxially grown graphene on SiC, focusing on growth kinetics, molecular orientation, structure and lattice parameters of pentacene on defect-free graphene. Epitaxially grown graphene on SiC possesses a high-quality crystal structure, essentially without grain boundaries. Pentacene thin films exhibit high structural order and relatively high field-effect mobility. The optical and electronic properties of pentacene are highly anisotropic. The films have been monitored in-situ with real-time X-ray scattering techniques (GISAXS, GIWAXS), ex-situ with atomic force microscopy (AFM) and polarized Raman measurements. Epitaxial growth of pentacene on graphene yields a lying-down molecular assembly that shows a six-fold symmetry with respect to graphene crystallographic orientation[1]. Surprisingly, the theoretical position of the 001 diffraction peak for the single crystal phase matches our thin film measurements. Temporal evolution of Rg reveals maximum value at 60 nm for 3 different substrate temperatures (320, 330, 350K).

[1] L. Wi Hyoung et al. Surface-Directed Molecular Assembly of Pentacene on Monolayer Graphene for High-Performance Organic Transistors. JACS 2011, (133), 4447.

CPP 15: Solid-liquid interfaces: Reactions and electrochemisty I (joint session O/CPP)

Time: Monday 15:00–16:30 Location: MA 144

CPP 15.1 Mon 15:00 MA 144

Towards size-selected supported Pd clusters in aqueous environment — •Nicolas Bock, Astrid de Clercq, Clara Rettenmaier, Ueli Heiz, and Friedrich Esch — Chemistry Department & Catalysis Research Center, Technische Universität München, Garching, 85747, Germany

Supported Palladium nanoparticles have been widely investigated as efficient electro- and photo-electro-catalysts. However, for the smaller sub-nanometer Pd clusters, little is known about their size-dependent catalytic properties and stability in aqueous environments. Since this non-scalable size regime bears the potential of high catalytic activity, we aim at finding new ways to prepare and study size-selected Pd clusters via controlled electrochemical decomposition.

To this purpose we have investigated the controlled decomposition of Pd-polyoxo-metalates [1] under specific electrochemical potential and pH conditions, taking advantage of their precise stoichiometry and redox properties. The investigation bases on Electrochemical Scanning Microscopy (ECSTM) and Rotating Disk Electrode (RDE) measurements. Reactivity measurements on single clusters using the STM tip as a microelectrode for hydrogen evolution monitoring are work in progress.

[1] P. Yang, Y. Xiang, Z. Lin, B. S. Bassil, J. Cao, L. Fan, Y. Fan, M.-X. Li, P. Jiménez-Lozano, J. J. Carbó, et al., Angewandte Chemie International Edition 2014, 53, 11974-11978.

CPP 15.2 Mon 15:15 MA 144

Probing ultrafast processes at electrode-aqueous solution interfaces with laser induced photovoltage measurements — •Yujin Tong, François Lapointe, Martin Wolf, and R. Kramer Campen — Fritz-Haber-Institut, Abt. Physikalische Chemie, 14195 Berlin, Germany

A conventional potentiostat that typically employed for a three electrode electrochemical system has a time resolution of, at best, 1 μ s (bandwidth above 1MHz) [Bard, A.J., Electrochemical methods: fundamentals and applications, New York: Wiley, (1980), Chapter 15]. However, many charge transfer processes happen on pico- to femtosecond time scales. To measure such fast kinetics, all-optical pump probe techniques using ultrafast lasers are usually adopted. In this contribution, we demonstrate that, using a sequence of two ultrashort laser pulses of different photon energies and detection of the laser induced photovoltage by a slow potentiostat as a function of the delay between the two incident pulses, ultrafast charge transfer kinetics on femtosecond timescales can be resolved. For example, we used a UV laser to trigger electron transfer from a gold electrode to Na_2SO_4 aqueous solution and then a second laser in middle or near infrared region was employed to interact with the species that generated by the freshly generated electron. The life time as well as the spectrum of the transient species is consistent with the solvated electron at the interface.

CPP 15.3 Mon 15:30 MA 144

The Reactivity of Individual 'Defect'-Sites on Electrochemically Roughened Pt(111) — •Leon Jacobse[1], Marcel J. Rost[2], and Marc T.M. Koper[1] — [1]Leiden Institute of Chemistry, Leiden University, Leiden, The Netherlands — [2]Huygens-Kamerlingh Onnes Laboratory, Leiden University, Leiden, The Netherlands

Platinum is arguably the most stable, highly active electrocatalyst under oxidizing conditions in acidic media. Nonetheless, the poorly understood electrode degradation process strongly limits the economic feasibility of large scale applications.

Previously, we have shown by combination of simultaneous cyclic voltammetry and in-situ EC-STM that the total electrochemical signal of Pt(111) is directly correlated to its surface roughness [1]. This analysis, however, did not yet provide a rationale for this correlation. A detailed analysis of the EC-STM images provides information on the atomic-scale structure of the formed Pt nano-islands and their evolution. Correlating the resulting density of specific surface sites to the different hydrogen adsorption features in the voltammetry, allows us to determine the electrochemical reactivity of formed step and kink sites on the roughened surface. This finally delivers an insight on how to describe the electrochemical reactivity not only of the observed nano-islands but also of Pt nanoparticles in general.

[1] L. Jacobse, Y.-F. Huang, M.T.M. Koper, M.J. Rost, Nature Materials, accepted (2017)

CPP 15.4 Mon 15:45 MA 144

Correlation of Surface Site Formation to Nano-Island Growth in the Electrochemical Roughening of Pt(111) — Leon Jacobse[1], Yi-Fan Huang[1], Marc Koper[1], and •Marcel Rost[2] — [1]Leiden Institute of Chemistry, Leiden University, Leiden, The Netherlands — [2]Huygens-Kamerlingh Onnes Laboratory, Leiden University, Leiden, The Netherlands

Platinum plays a central role in a wide variety of electrochemical devices. Electrode degradation, especially under oxidizing conditions, forms an important barrier for the widespread of applications. Although it is known that repeated oxidation and reduction of platinum electrodes results in irreversible surface structure changes, over thirty years of research did not yet yield to a conclusive description of this process on the atomic level; even not for well-defined single crystal surfaces.

Using a special EC-STM, which is capable of measuring the electrochemical signals simultaneously during imaging in operando, we directly correlate, for the first time, the evolution of the hydrogen adsorption peaks on Pt(111) to the observed roughening of the surface. In the later stages, we find a strong correlation between the evolution of the roughness and the absorption peaks clearly indicating that each created step contributes equally strong to the adsorption signal as well as to the roughness. However, and fully surprising, in the early stage step edges are created that seem to be chemically "dead".

CPP 15.5 Mon 16:00 MA 144

Driving hyrodrogen evolution and oxidation on Pt with femtosecond laser pulses — •Gregor Zwaschka, Yujin Tong, Martin Wolf, and R. Kramer Campen — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

The Hydrogen Evolution and Oxidation Reactions (HER/HOR) on Pt have been studied for decades due to their fundamental interest and importance in applications such as electrolyzers and fuel cells. Despite much effort there is no clear view of the mechanism of these reactions that can explain the large dependence of their rates on surface structure, pH and electrolyte. Because the HER/HOR on Pt are fast, one possible explanation for the challenge in obtaining such mechanistic insight is that intermediates exist on the Pt electrode surface at very low concentrations under steady state reactive conditions. In principle such a limit can be overcome by rapidly and transiently increasing the amount of reactants present and characterizing their effect. Here we present our efforts to trigger the HER/HOR on Pt using femtosecond laser pulses. The resulting, laser-induced voltammogram clearly shows that the femtosecond pulse train induces HER/HOR and that the magnitude of this effect depends on crystal face in a manner rationalizable by the surface electronic structure. Control experiments varying pulse lengths, energies and the frequencies of the incident field suggest that we induce the HER/HOR by creating a population of hot electrons. Theses results offer a novel experimental window on the HER/HOR and are a first step in experimentally characterizing the mechanisms of these important reactions.

CPP 15.6 Mon 16:15 MA 144

On-surface synthesis of covalent architectures for energy conversion chemistry — •Patrick Alexa[1], Doris Grumelli[2], Diana Hötger[1], Vjay Vias[3], Bettina Lotsch[1,4], Rico Gutzler[1], and Klaus Kern[1,5] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Universidad Nacional de La Plata, 1900 La Plata, Argentina — [3]Marquette University, Milwaukee, WI 53233, USA — [4]University of Munich (LMU), 81377 Munich, Germany — [5]Ecole Polytéchnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Creating nanostructures in a bottom-up approach by using molecular precursors allows for the fabrication of tailored nanomaterials for specific applications such as energy conversion. In particular (metal)organic networks synthesized in UHV on crystalline surfaces can be used as efficient electrocatalysts. Inspired by the photocatalytic hydrogen evolution properties of triazine-containing bulk covalent organic frameworks, we investigate structurally similar 2D networks for their propensity for the hydrogen evolution reaction. In this work we synthesize two-dimensional covalent polymers from 2,4,6-tri-(4-bromophenyl)-1,3,5-triazine on Au(111) and visualize their topography by scanning tunneling microscopy. The polymer-decorated surface shows a promising improvement for the hydrogen evolution reaction compared to bare Au(111) in electrocatalytic experiments. The influence of electrolyte exposure and electrocatalytic conditions on the polymer structure is discussed. These results highlight the capability of single-layer functional 2D polymers for electrocatalysis.

CPP 16: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials II (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Monday 15:00–17:15 Location: HL 001

CPP 16.1 Mon 15:00 HL 001

Non-adiabatic Dynamics in Single-Electron Tunneling Devices with Time-Dependent Density Functional Theory — •Niklas Dittmann[1,2,3], Janine Splettstoesser[2], and Nicole Helbig[3] — [1]Institute for Theory of Statistical Physics, RWTH Aachen University, Germany — [2]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Gothenburg, Sweden — [3]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

The recent advance of various single-electron sources in solid-state setups has sparked interest in the investigation of electronic transport at the single-particle level. In our recent work (N. Dittmann, J. Splettstoesser, N. Helbig, arxiv:1706.04547), we put forward time-dependent density-functional theory to calculate the dynamics of interacting electrons in single-electron tunneling devices. As a physical system, we analyze a single-electron source which is built by a quantum dot tunnel-coupled to a nearby electron reservoir and driven by a time-dependent gate voltage. By using analogies with quantum-transport theory, we extract a time-nonlocal exchange-correlation potential for a Hubbard U on-site interaction on the quantum dot. The time nonlocality manifests itself in a dynamical potential step, which we explicitly link to physical relaxation time scales of the electron dynamics. Finally, we discuss prospects for simulations of larger mesoscopic systems.

CPP 16.2 Mon 15:15 HL 001

Dissipative exchange-correlation functional in QED-TDDFT — •Camilla Pellegrini[1], Ilya Tokatly[2,3], and Angel Rubio[2,4] — [1]Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, E-20018 San Sebastian, Spain — [3]IKERBASQUE, Basque Foundation for Science, 48001 Bilbao, Spain — [4]Max Planck Institute for the Structure and the Dynamics of Matter, Luruper Chausse 149, 22761 Hamburg, Germany

Time-dependent density functional theory has been recently extended to treat many-electron systems coupled to quantized electromagnetic modes. Here we discuss the implications of this approach for the theory of open quantum systems. In particular we show that in the limit of continuous spectrum of photon modes, QED-TDDFT naturally leads to time-dependent density functional theory for dissipative systems coupled to the Caldeira-Leggett bath. We consider the application to the Ohmic spin boson model and show that the developed approximation to the exchange-correlation functional describes the natural linewidth of the electronic linear density response function.

CPP 16.3 Mon 15:30 HL 001

Electric and magnetic response properties of solids from the current density — •Rubén Rodríguez Ferradás[1], Pina Romaniello[2], and Arjan Berger[1] — [1]LCPQ, University of Toulouse, France — [2]LPT, University of Toulouse, France

The evaluation of the macroscopic polarization and magnetization of solids is problematic when periodic boundary conditions are used because surface effects are artificially removed. This poses a problem unless surface effects can be reformulated in terms of bulk quantities [1-5]. In this work we show the advantage of calculating electric and magnetic response properties of solids using the current density as basic variable. An efficient approach to calculate the current density is time-dependent current-density-functional theory. We will show results for optical properties of solids using a recently developed functional [6]. We will also discuss how the magnetization can be described within this framework.

[1] F. Kootstra, P.L. de Boeij, and J.G. Snijders, J. Chem. Phys. 112, 6517.

[2] J.A. Berger, P.L. de Boeij, and R. van Leeuwen, Phys. Rev. B 71, 155104 (2005).

[3] P. Romaniello and P.L. de Boeij, Phys. Rev. B 71, 155108 (2005).

[4] J.A. Berger, P. Romaniello, R. van Leeuwen, and P.L. de Boeij, Phys. Rev. B 74, 245117 (2006).

[5] J.A. Berger, P.L. de Boeij, and R. van Leeuwen, Phys. Rev. B 75, 035116 (2007).

[6] J.A. Berger, Phys. Rev. Lett. 115, 137402 (2015)

CPP 16.4 Mon 15:45 HL 001

Coupling Maxwell's equations to the time-dependent Kohn-Sham equations: near-field effects and electromagnetic backreaction — •Rene Jestaedt[1], Micael Oliveira[1], Angel Rubio[1,2,3], and Heiko Appel[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, USA — [3]Nano-bio Spectroscopy Group and ETSF, Universidad del País Vasco, 20018 San Sebastián, Spain

Induced currents in large molecular and condensed matter systems are non-negligible and can affect the conductivity and the optical properties of the system. In the present work, we have implemented the real-time propagation of Maxwell's equations in Riemann-Silberstein representation to use standard unitary propagation techniques in the TDDFT code octopus [1]. The Maxwell and the Kohn-Sham system are coupled via a predictor-corrector method to obtain a self-consistent time-evolution of the total system [2]. Explicitely solving the microscopic Maxwell's equations also allows us to determine the optical properties of the system directly from the Maxwell fields. We show near-field effects of a full Maxwell-matter and matter-Maxwell coupling for plasmon excitations in metallic nanoparticles [2,3] and for ring-currents in organic molecules [2].

[1] Alejandro Varas et al., J. Phys. Chem. Lett. 2015, **6**, 1891-1898 / [2] R. Jestädt et al., (to be submitted) / [3] X. Andrade et al., Physi. Chemistry Chem. Physics 2015, **17** 31371-31396

CPP 16.5 Mon 16:00 HL 001

Enhancing excitation energy and charge transfer with strongly correlated light-matter interaction — •Christian Schäfer[1], Michael Ruggenthaler[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

Förster excitation energy and charge transfer are fundamental processes of chemical reactions and connected to interesting quantities such as correlation. Often this correlation is taken as fixed property of the system.

In the current work, we present how the coupling to cavity photons in a minimal realistic molecular system can drastically alter transfer characteristics, e.g. renders the excitation transfer to be distance independent [1,2]. The photonic interaction can imprint fermionic correlation on arbitrary distances.

The exact real-space description is suited to describe transfer and correlation in a unprejudiced ab-initio picture and allows us to extend our insights beyond common quantum-optical approximations.

[1] X. Zhong et al., Angew Chem Int Ed Engl. **56(31)**, 9034 (2017). [2] M. Slootsky et al., PRL **112**, 076401 (2014).

CPP 16.6 Mon 16:15 HL 001

Effects of electronic correlations on the magnetic properties of organometallic molecules — •Sumanta Bhandary and Silke Biermann — Centre de Physique Thèorique, Ecole Polytechnique, 91128 Palaiseau, France

The realm of molecular spintronics relies on the external accessibility of molecular magnetic states. In correlated organometallic complexes, a delicate balance between the crystal field, Coulomb repulsion and dynamical hybridization between metal center and organic ligands dictates the electronic and magnetic properties and often poses challenges for an accurate theoretical modelling. We have employed density functional theory (DFT), the GW approach and Anderson's impurity model (AIM) technique to study the ground state electronic and magnetic properties of transition metal-based porphyrin and phthalocyanine molecules, both in the gas phase [1] as well as while adsorbed on surfaces. Our study reveals that the dynamical correlation effects are important in order to accurately estimate spin-transition energies, magnetic anisotropy energies as well as the ground state electronic configurations in the molecular complexes. We have explored the manipulation of surface molecule interactions to externally influence the electronic and magnetic properties of the molecular system.

[1] S. Bhandary, M. Schüler, P. Thunström, I. di Marco, B. Brena, O. Eriksson, T. Wehling, and B. Sanyal, Phys. Rev. B **93**, 155158 (2016).

CPP 16.7 Mon 16:30 HL 001

Structural, electronic and optical properties of cubic and tetragonal SrTiO$_3$: a DFT study including many-body effects — •Vijaya Begum, Markus E. Gruner, and Rossitza Pentcheva — Faculty of Physics and Centre for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg.

SrTiO$_3$ (STO) is of fundamental interest as a substrate material in oxide electronics. The bulk undergoes a phase transition from the cubic to a tetragonal structure at T=105 K accompanied by characteristic antiferrodistortive rotations of the TiO$_6$ octahedra. We present a systematic comparison of the performance of the gradient corrected exchange correlation functional (GGA), the strongly constrained and appropriately normed (SCAN) meta-GGA and the hybrid functional HSE06 with respect to the electronic, structural and optical properties of cubic and tetragonal STO. For the tetragonal structure, SCAN gives a significantly improved description of the structural properties, comparable to HSE06, at a computational cost similar to GGA. The experimental band gap can be reproduced within SCAN with an on-site Hubbard term (+U), whereas within GGA the gap is underestimated even for very high U values. We calculate the optical spectrum for both phases, including many-body effects and excitonic corrections within the GW+Bethe-Salpeter equation approach, and compare this to previous theoretical results for the cubic phase [PRB 87, 235102 (2013)] and experiment [PRB 93, 075204 (2016)]. Funding by the DFG within SFB1242, project C02 is gratefully acknowledged.

CPP 16.8 Mon 16:45 HL 001

Unveiling the mysterious magnetic state of superconducting iron under pressure — •Matteo d'Astuto — Institut NEEL CNRS/UGA UPR2940 25 rue des Martyrs BP 166 38042 Grenoble cedex 9 FRANCE — IMPMC, UMR CNRS 7590, Sorbonne Universités-UPMC University Paris 06, MNHN, IRD, 4 Place Jussieu, F-75005 Paris, France

Compressed iron undergoes a transition from bcc to hcp crystal structure with a loss of ferromagnetism. The magnetic state of the hcp phase has been debated for many decades and experiments give seemingly contradictory results. Mössbauer measurements find no magnetism, however x-ray emission spectroscopy finds remnant magnetism and Raman mode splitting suggests symmetry breaking due to antiferromagnetism. These paradoxical results are consistent with either a paramagnetic state with spin fluctuations faster than Mössbauer timescales or an antiferromagnetic state, afmII, which is undetectable with Mössbauer spectroscopy. We performed neutron powder diffraction measurements in the hcp phase and do not observe afmII order down to 1.8 K, while confirming the existence of a local magnetic moment in the hcp phase with x-ray emission spectroscopy and find it is intrinsic to this phase (1). This local magnetic moment disappears at 30–40 GPa, exactly the same pressure region where superconductivity disappears.

(1) B. W. Lebert, T. Gorni J.-P. Rueff, S. Klotz, M. Casula, A. Juhin, J. M. Ablett, F. Baudelet, T. Straessle, T. Hansen, A. Polian, P. Munsch, G. Le Marchand, Z. Zhang, M. d'Astuto, article in preparation.

CPP 16.9 Mon 17:00 HL 001

Frist-principle and experimental characterisation of the electronic properties of CaGaSiN3 and CaAlSiN3: impact of chemical disorder — •Jan Minar[1], Ondrej Sipr[2], Robin Niklaus[3], Jonas Hausler[3], and Wolfgang Scgnick[3] — [1]New Technologies Research Center, University of West Bohemia, Pilsen, Czech Rep., — [2]FZU, Academy of Sciences, Czech Rep — [3]Department of Chemistry, University of Munich, Munich, Germany

We report a detailed investigation of the electronic, mechanical and optical properties of the recently discovered nitridogallosilicate CaGaSiN3 which has potential as a LED-phosphor host material. We focus on chemical disorder effects, originating from the Ga/Si site, and compared them to those of isostructural CaAlSiN3. We calculate the elastic moduli and the Debye temperature in terms of quasi harmonical approximation. Spectral properties like the joint density of states (JDOS) are evaluated and the absorption, reflectance and energy loss function are obtained from the dielectric function. The optical band gap of CaGaSiN3 from experiment is compared to the electronic band gap in terms of electronic DOS and band structure calculations. All properties are evaluated for different ordering models of Ga/Si while the experimentally observed substitutional disorder is accounted for by utilizing the Coherent Potential Approximation (CPA). We conclude a shrinking of the band gap for both CaGaSiN3 and CaAlSiN3 due to atomic disorder, which is unfavorable for potential phosphor applications [1]. R. Niklaus, J. Minar, J Häusler, W. Schnick, Physical Chemistry Chemical Physics 19 (13), 9292 (2017)

CPP 17: Active Matter II (joint session DY/CPP/BP)

Time: Monday 15:30–18:45 Location: BH-N 243

CPP 17.1 Mon 15:30 BH-N 243

Run-and-Tumble-like Motion of Synthetic Microswimmers in Viscoelastic Media — •Celia Lozano, J. Ruben Gomez-Solano, and Clemens Bechinger — Fachbereich Physik, Universität Konstanz, Konstanz D-78457, Germany

Run-and-tumble (RNT) motion is a prominent locomotion strategy employed by many living microorganisms. It is characterized by straight swimming intervals (runs), which are interrupted by sudden reorientation events (tumbles). In contrast, directional changes of synthetic microswimmers (active particles, APs) are caused by rotational diffusion, which is superimposed with their translational motion and, thus, leads to rather continuous and slow particle reorientations. Here we demonstrate that APs can also perform a swimming motion where translational and orientational changes are disentangled, similar to RNT. In our system, such motion is realized by a viscoelastic solvent and a periodic modulation of the self-propulsion velocity. Experimentally, this is achieved using light-activated Janus colloids, which are illuminated by a time-dependent laser field. We observe a strong enhancement of the effective translational and rotational motion when the modulation time is comparable to the relaxation time of the viscoelastic fluid. Our findings are explained by the relaxation of the elastic stress, which builds up during the self-propulsion, and is suddenly released when the activity is turned off. In addition to a better understanding of active motion in viscoelastic surroundings, our results may suggest novel steering strategies for synthetic microswimmers in complex environments.

CPP 17.2 Mon 15:45 BH-N 243

Effective viscosity of active suspensions — Levan Jibuti[1], Walter Zimmermann[1], Salima Rafai[2], and •Philippe Peyla[2] — [1]Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany — [2]LIPhy, Université Grenoble Alpes and CNRS, F-38402 Grenoble, France

Micro-organisms usually can swim in their liquid environment by flagellar or ciliary beating. In this numerical work, we analyze the influence of flagellar beating on the orbits of a swimming cell in a shear flow. We also calculate the effect of the flagellar beating on the rheology of a dilute suspension of microswimmers. A three-dimensional model is proposed for Chlamydomonas Reinhardtii swimming with a breaststroke-like beating of two anterior flagella modeled by two counter-rotating fore beads. The active swimmer model reveals unusual angular orbits in a linear shear flow. This peculiar behavior has some significant consequences on the rheological properties of the suspension. We calculate Einstein's viscosity of the suspension composed of such isolated modeled microswimmers (dilute case) in a shear flow. The results show an increased intrinsic viscosity for active swimmer suspensions in comparison to nonactive ones as well as a shear thinning behavior in accordance with our previous experimental measurements.

Effective viscosity of a suspension of flagellar-beating microswimmers: Three-dimensional modeling Levan Jibuti, Walter Zimmermann, Salima Rafaï, and Philippe Peyla Phys. Rev. E 96, 052610 (2017)

CPP 17.3 Mon 16:00 BH-N 243

Self propulsion of droplets driven by an active permeating gel — •Reiner Kree and Annette Zippelius — Inst. f. Theoret. Physik, Univ. Göttingen, Friedrich-Hund. Pl. 1, 37077 Göttingen

We discuss the flow field and velocity of active droplets, which are driven by body forces residing on a rigid gel. The latter is modeled as a porous medium which gives rise to permeation forces. In the simplest model, the Brinkmann equation, the porous medium is characterized by a single length scale l, the square root of the permeability. We compute the flow fields, the translational and rotational velocity of the droplet and the energy dissipation as a function of l. We show that the model gives rise to non-monotic behaviour of the droplet velocities and the dissipated power as functions of the gel fraction. As l changes from large to small values, the properties of the medium change from a simple viscous fluid to a Darcy medium. We discuss the behaviour of flow, velocities and force densities as these limits are approched.

CPP 17.4 Mon 16:15 BH-N 243

Viscotaxis: a theory for microswimmer navigation in viscosity gradients — •Benno Liebchen[1], Paul Monderkamp[1], Borge ten Hagen[2], and Hartmut Loewen[1] — [1]Institut fuer Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universitaet Duesseldorf, D-40225 Duesseldorf, Germany — [2]Physics of Fluids Group, Faculty of Science and Technology, University of Twente, 7500 AE Enschede, The Netherlands

The survival of many microorganisms, like Leptospira or Spiroplasma bacteria, which swim poorly in low-viscosity fluids, depends on their ability to navigate up viscosity gradients. While this ability, called viscotaxis, has been observed in several experiments with microorganisms, the underlying mechanism remains unclear. In the present talk, we present a simple theory for viscotaxis of self-propelled swimmers [1] in slowly varying viscosity gradients: this theory unveils specific mechanisms for viscotaxis based on a systematic imbalance of viscous forces acting on different body parts of a swimmer and allows to classify microswimmers regarding their ability to perform viscotaxis based on their body shapes. Besides shedding new light on microorganism viscotaxis, our results may be useful to design synthetic swimmers with the ability to navigate in viscosity gradients (akin to synthetic chemo- or thermotactic swimmers [2]).

[1] B. Liebchen, P. Monderkamp, B.t. Hagen and H. Löwen, in preparation.

[2] B. Liebchen, D. Marenduzzo, and M. E. Cates, Phys. Rev. Lett. 118, 268001 (2017).

CPP 17.5 Mon 16:30 BH-N 243

Photo-gravitaxis in synthetic microswimmers — •William Uspal[1,2], Dhruv Singh[1], Mihail Popescu[1,2], Laurence Wilson[3], and Peer Fischer[1,4] — [1]Max-Planck-Institut für Intelligente Systeme — [2]IV. Institut für Theoretische Physik, Universität Stuttgart — [3]Department of Physics, University of York — [4]Institut für Physikalische Chemie, Universität Stuttgart

We study the dynamics of active Janus particles that self-propel in aqueous solution by light-activated catalytic decomposition of chemical "fuel." In experiments, the particles, initially sedimented at a bottom wall, exhibit wall-bound states of motion, dependent on the size of the particle, when illuminated from underneath the wall. Upon increasing the intensity of the light above a threshold value, which is also dependent on the size of the particle, the particles lift off the wall and move way from it, i.e., they exhibit a photo-gravitactic behavior similar to some planktonic microorganisms. The dependencies on the particle size are rationalized by using a theoretical model of self-phoresis that explicitly accounts for the "shadowing" effect of the opaque catalytic face of the particle. Our model allows us to unequivocally identify the photochemical activity and phototactic response as the key mechanisms beyond the observed phenomenology. Consequently, one has the means to design photo-gravitatic particles that can reversibly switch between operating near a boundary or in the volume away from the boundary by judiciously adjusting the light intensity, i.e., simply by "turning a knob".

15 min. break

CPP 17.6 Mon 17:00 BH-N 243

Active Rods in a Converging Flow — •Andreas Kaiser[1], Mykhailo Potomkin[2], Leonid Berlyand[2], and Igor Aranson[1,2] — [1]Department of Biomedical Engineering, Pennsylvania State University, University Park, 16802, USA — [2]Department of Mathematics, Pennsylvania State University, University Park, 16802, USA

We consider active rodlike particles swimming in a convergent fluid flow in a trapezoid nozzle by using mathematical modeling to analyze trajectories of these particles inside the nozzle and numerical simulations to show that trajectories are strongly affected by the background fluid flow and geometry of the nozzle leading to wall accumulation and rheotaxis. We describe the non-trivial focusing of active rods depending on physical as well as geometrical parameters. It is also established that the convergent component of the background flow leads to stability of both downstream and upstream swimming at the centerline. The stability of downstream swimming enhances focusing, and the stability of upstream swimming enables rheotaxis in the bulk.

CPP 17.7 Mon 17:15 BH-N 243

Guidance of self-phoretic Janus particles by chemically patterned surfaces — William Uspal[1,2], •Mihail Popescu[1,2], Mykola Tasinkevych[3], and Siegfried Dietrich[1,2] — [1]M.P.I. for Intelligent Systems, Stuttgart, Germany — [2]University of Stuttgart, Germany — [3]University of Lisbon, Portugal

Self-phoretic Janus particles move by inducing – via non-equilibrium chemical reactions occurring on their surfaces – gradients in chemical composition along the surface of the particle, as well as along any nearby boundaries. The chemical gradients along a wall can give rise to chemi-osmosis, which, in turn, drives flow in the volume of the solution and thus couples back to the particle. This response flow induced and experienced by a particle encodes information about any chemical patterning of the wall. Here, we show by analytical calculations, complemented with numerical solution, that wall-patterning by chemical steps can provide the means for docking of achieving a step-guided motion of such an active particle, and we discuss the dependence of the phenomenology on the shape (spherical or rod-like) of the particle. Furthermore, we show that such chemically active particles in general align with, and follow, spatial gradients in the surface chemistry of the wall (i.e., they exhibit thigmo-taxis).

CPP 17.8 Mon 17:30 BH-N 243

Randomly shaped magnetic Micropropellers — •Felix Bachmann[1], Agnese Codutti[1,2], Klaas Bente[1], and Damien Faivre[1] — [1]Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Science Park Golm — [2]Max Planck Institute of Colloids and Interfaces, Department of Theory & Bio-Systems, Science Park Golm

Over the last decade many different actuation mechanisms for swimming at low Reynolds number have been suggested and implemented. Magnetic micropropellers are a promising example that combines remote and fuel-free actuation with precise control. Now, the realization of the envisioned, mostly medical application is the next step. Therefore, automation and additional control strategies have to be developed. In this regard, randomly shaped micropropellers offer the possibility to find and test new actuation schemes and the associated propeller shapes. We screen a pool of such randomly shaped magnetic micropropellers by applying different magnetic fields and record their swimming behavior by optical high speed microscopy, which additionally enables tomographic 3D-shape reconstructions of interesting propellers. This is the basis for their reproduction through micro- and nanofabrication and eventually facilitates the formulation of micropropeller design guidelines for special applications.

CPP 17.9 Mon 17:45 BH-N 243

Active Brownian particles in a inhomogeneous activity or magnetic field — •Hidde Vuijk and Abhinav Sharma — Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, 01069 Dresden

We study spherically symmetric active particles in a spatially inhomogeneous activity or magnetic field. In both cases the particles spontaneously orient themselves, which results in an inhomogeneous distribution of particles. Using Green-Kubo approach we obtain analytical expression for the orientation of the particles. We find that the relevant equilibrium correlation function is the self-part of the Van Hove function, which can be approximated accurately. Density does not have a linear response to the activity; however, an expression for the density is derived by using the orientation as input to dynamic density functional theory. All theoretical predictions are validated using Brownian dynamics simulations.

CPP 17.10 Mon 18:00 BH-N 243

Active colloidal particles in evaporating liquid droplets — •Borge ten Hagen[1], Maziyar Jalaal[1], Hai Le The[2], Christian Diddens[1], Alvaro Marin[1], and Detlef Lohse[1,3] — [1]Physics of Fluids Group and Max Planck Center Twente, University of Twente, Enschede, The Netherlands — [2]MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands — [3]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Inspired by biological microswimmers, various types of artificial self-propelled particles have been developed and thoroughly characterized in recent years. While in most studies quiescent solvents or stationary flow fields were considered, much less is known about the behavior of synthetic microswimmers in more complicated flow environments as they often occur in biological systems under non-laboratory conditions. Here, we investigate the dynamics of self-propelling Janus particles in an evaporating droplet of hydrogen peroxide solution. The competition between the flows due to the evaporation and the active motion of the particles leads to a complex dynamical behavior. The system is analyzed using three-dimensional particle tracking measurements and numerical simulations of the nontrivial fluid flow within the evaporating droplet. It will also be discussed how the particle activity affects the coffee-ring formation in the final state of evaporation, where the orientation of the Janus particles introduces a new order parameter.

CPP 17.11 Mon 18:15 BH-N 243

Active droplet model of cellular aggregates — •Hui-Shun Kuan, Frank Jülicher, and Vasily Zaburdaev — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Active systems appear in various biological contexts such as cell cytoskeleton and bacterial colonies. Such systems may exhibit phase separation, which is not governed by free energy minimization. In this talk, we use the concept of phase separation to study the formation of bacterial colonies, of N. gonorrhoeae, due to active force generation by cell appendages type IV pili. We use a hydrodynamics approach, representing bacterial colonies as active droplets, which exhibit different surface profiles and position-dependent motility gradients. In addition, the coalescence of two such droplets exhibits two time scales which cannot be understood by the surface tension and viscosity. Our theoretical description of active droplets provides means of describing bacterial colonies and can be extended to other cell types.

CPP 17.12 Mon 18:30 BH-N 243

3D dynamics of synthetically assembled microtubules and motors — •Smrithika Subramani, Christian Westendorf, Eberhard Bodenschatz, and Isabella Guido — Max Planck Institute for dynamics and self-organization, Göttingen, Germany

Cytoskeletal filaments such as microtubules play a major role in cell division, organelle transport and cellular motility. These diverse biological functionalities are driven by bending, looping and buckling of microtubule (MT) filaments. In our study, we intend to gain a deeper understanding of these phenomena by synthetically reconstituting dynamic MT structures.

We hierarchically build a model active matter system using depletion-driven MT bundles and the processive motor Kinesin-1, assembled in a tetrameric complex. By hydrolyzing ATP and undergoing a conformational change, the motor complex is able to effectively 'walk' along MT bundles and generate motion in a 3D environment. Our observations include continuous sliding, bending and buckling of MT bundles into long-wavelength arcs, resembling their in vivo behaviour. By using the Fluorescence Recovery After Photobleaching (FRAP) method, we are able to analyze the MT structure distribution. A multi-plane fluorescence microscopy technique enables us to observe the bundle dynamics in 3D.

CPP 18: Focus: Droplets (joint session DY/CPP)

The physics of droplets is surprisingly rich - and full of surprises. This holds for droplets in ambient gas and for droplets in other liquids. The geometric and dynamical parameters which enter are size and velocity and the material properties are density, surface tension, velocity, volatility, freezing and melting points, latent heat, viscosity, thermal conductivity,... and all this holds for both the drops and for the surrounding gas or liquid. Moreover, both droplet and surrounding can be multicomponent and phase transitions and chemical reactions. The consequence of this huge parameter space is a plethora of often very surprising phenomena - and many are technologically very important. The systematic optimization of processes involving such phenomena needs a fundamental understanding of the physics. In this session various examples are given in which the community has worked towards such an understanding, combining controlled experiments, numerical simulations, and theoretical analysis.

D. Lohse

Time: Monday 15:30–19:15 Location: BH-N 334

CPP 18.1 Mon 15:30 BH-N 334

Marangoni Contraction of Evaporating Sessile Droplets of Binary Mixtures — •Stefan Karpitschka[1], Ferenc Liebig[2], and Hans Riegler[3] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen — [2]Institute of Chemistry, University of Potsdam, Karl-Liebknecht-Straße 24-25, 14476 Potsdam — [3]Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14476 Potsdam

The evaporation of sessile droplets of mixtures is a ubiquitous natural and industrial process, relevant, e.g., for cleaning/drying of semiconductor surfaces or for ink-jet printing. For binary mixtures, the component with the higher vapor pressure will usually evaporate faster and thus deplete from the contact line region of a droplet. In general, different liquids have different surface tensions. Thus, evaporation causes surface tension gradients and Marangoni flows. Here we investigate the impact of evaporation on the wetting behavior of binary mixtures [Langmuir 33, 4682 (2017)]. We measure non-zero apparent contact angles even if both liquid components individually wet the substrate completely. Simulations show that the interplay of Marangoni flow, capillary flow, diffusive transport, and evaporative losses can establish a quasi-stationary drop profile with an apparent nonzero contact angle. In good agreement with experiments, we reveal a previously unknown universal power-law relation between the apparent contact angle and the relative undersaturation of the atmosphere, which can be inferred from the scaling analysis of the hydrodynamic-evaporative evolution equations.

CPP 18.2 Mon 15:45 BH-N 334

Equilibrium versus non-equilibrium positioning of droplets — •Samuel Krüger[1,2], Christoph A. Weber[4], Jens-Uwe Sommer[2,3], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Leibniz Institute of Polymer Research Dresden e.V — [3]Technische Universität Dresden, Institute of Theoretical Physics, Dresden, Germany — [4]Division of Engineering and Applied Sciences, Harvard University, Cambridge, USA

The position of droplets can be controlled by concentration gradients of a component which affect phase separation. A concentration gradient can be generated by an external potential or by boundary conditions. While systems with external potentials belong to the class of equilibrium systems, applying boundary conditions corresponds to a non-equilibrium scenario. We aim to understand what is the difference between these two scenarios and how the positioning is affected. To this end, we consider a ternary system where two components phase separate while a third component regulates their phase separation. We use Monte-Carlo simulations to compare the positioning of droplets between the two scenarios. In both scenarios we find that the droplet is positioned toward the region of low or high regulator concentration depending on their interaction parameters. The essential differences are the set of interaction parameter where the switch of position occurs. The positioning of droplets is relevant in cells prior to cell division or applications in microfluidic devices such as aqueous computing.

CPP 18.3 Mon 16:00 BH-N 334

Drying Teardrops — •Alvaro Marin[1], Stefan Karpitschka[2], Christian Diddens[3], Massimiliano Rossi[4], Christian J. Kähler[4], Diego Noguera-Marin[5], and Miguel A. Rodriguez-Valverde[5] — [1]Max Planck + University of Twente Center for Complex Fluid Dynamics, The Netherlands — [2]Max Planck Center for Dynamics and Self-Organization, Germany — [3]Physics of Fluids, University of Twente, The Netherlands — [4]Bundeswehr University Munich, Neubiberg, Germany — [5]Biocolloid and Fluid Physics group, University of Granada, Spain

Salt can be found in different forms in almost any evaporating droplet in nature, our homes and in our own tears. Dried teardrops present an amazing variety of forms, shapes and crystals (even for the same person), but they all have something in common: a ring-shaped stain. In this talk we will address a model teardrop system consisting of an evaporating water sessile droplet with sodium chloride concentrations from 1 mM up to 100 mM. With experimental measurements and numerical simulations we can show that the transport of liquid in this system differs strongly from 'sweet' evaporating water droplets: the liquid flows in the inverse direction due to strong Marangoni stresses at the surface. Such an effect has crucial consequences to the deposition of salt, its crystallization and to the formation of the ring-shaped stains. In summary, our aim is to show that other mechanisms different than the famous "coffee-stain effect" can yield ring-shaped stains in evaporating sessile droplets.

CPP 18.4 Mon 16:15 BH-N 334

Protein Interactions Control Dynamics Of Liquid Compartments — •Tyler S. Harmon[1,2], Anthony A. Hyman[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Max Planck Institute for the Physics of Molecular Cell Biology, 01307 Dresden, Germany

Membraneless organelles form in cells due to liquid-liquid phase separation and have been implicated in a range of functions. The physical properties of these compartments are important for their function and thus should be tuned to match their intended purpose. Multiple diseases are associated with a hardening transition where these liquid compartments transition from a functional liquid-like state to an aberrant solid-like state over a long period of time. Other compartments appear to be designed to mature naturally from a liquid into a more solid compartment. Therefore, the physical mechanism controlling the liquid to solid transition is at the heart of how cells regulate and control these compartments.

We designed a three-dimensional polymer lattice model to investigate mechanisms for hardening in liquid compartments. We explore several mechanisms affecting the time dependence of protein dynamics. This allows us to test which protein properties are important for controlling the slowing of the dynamics of the liquid compartments. We analyzed the transition to a solid-like state by quantifying the time dependence of diffusion rates, density, and reversibility of dissolution. These results are a promising first step to reach a molecular picture of the hardening process.

CPP 18.5 Mon 16:30 BH-N 334

Oscillatory wetting under drops impacting on a hot plates — •Kirsten Harth, Michiel A. J. van Limbeek, Chao Sun, Andrea Prosperetti, and Detlef Lohse — Physics of Fluids, Max Planck Center for Complex Fluid Dynamics and University of Twente, The Netherlands

The Leidenfrost phenomenon, where an evaporating drop levitates above a layer of its vapour on sufficiently hot plates is well-known for gently deposited drops. For impacting drops, the additional impact pressure can cause much thinner vapour layers in the nanometer range, and conventional side or bottom view imaging is incapable of detecting substrate contact. Using frustrated total internal reflection (FTIR), three main regimes were distinguished: contact, nucleate boiling at low temperatures (drop spreads in contact with substrate), Leidenfrost (film) boiling without contact and a broad transition regime. Then, the outer parts of the spreading lamella levitate, while the central region of the drop touches the substrate. However, the wetted locations and the drop's partially levitated bottom surface increasingly fluctuate with increasing temperature. Most striking are periodic waves travelling from the lamella tips toward the centre of the wetted region. We analyze and discuss this currently unresolved phenomenon.

CPP 18.6 Mon 16:45 BH-N 334

Spontaneous jumping, bouncing and trampolining of hydrogel drops on a heated plate — •Doris Vollmer[1], Jonathan Pham[1], Sanghyuk Wooh[1], Tadashi Kajiya[1,2], and Hans-Jürgen Butt[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Analysis Technology Center, Fujifilm, Nakanuma, Japan

We study the dynamics of hydrogel drops, i.e. sold drops containing up to 97% of water. Using high speed video microscopy, we demonstrate that hydrogel drops, initially at rest on a surface, spontaneously jump upon rapid heating and continue to bounce with increasing amplitudes. Jumping is governed by the surface wettability, surface temperature, hydrogel elasticity, and adhesion. A combination of low adhesion impact behavior and fast water vapor formation supports continuous bouncing and trampolining. Our results illustrate how the interplay between solid and liquid characteristics of hydrogels results in intriguing dynamics, as reflected by spontaneous jumping, bouncing, trampolining, and extremely short contact times.

J.T. Pham, M. Paven, S. Wooh, T. Kajiya, H.-J. Butt, D. Vollmer, Nat. Comm., 2017, 8, 905

15 min. break

CPP 18.7 Mon 17:15 BH-N 334

Droplets in moist Rayleigh-Bènard convection — Prasanth Prabhakaran, Alexei Krekhov, •Stephan Weiss, and Eberhard Bodenschatz — Max Planck Institute f. Dynamics and Self-Organisation, Göttingen, Germany

We report experiments on condensation patterns in a moist Rayleigh-Bénard convection experiment. We use Sulphur Hexaflouride (SF_6) at high pressure as the working fluid and the experiment is operated across the liquid-vapor coexistence line close and far from the critical point. A layer of liquid SF_6 forms at the warm bottom of the cell. From its surface, vapor evaporates and condenses at the cold top plate, where it forms a thin film that undergoes a Rayleigh-Taylor like instability. As a result droplets form due to pinch-off that fall back into the liquid layer. Depending on the pressure and the temperature difference between bottom and top, locations where droplet form can lie on an almost stationary hexagonal grid with a well defined wavelength. When the liquid level at the bottom plate is eliminated the droplets falling from the top plate levitate above the bottom plate due to Leidenfrost effect. Under appropriate conditions the Leidenfrost drops form large domains with multiple chimneys (multi-connected domains).

CPP 18.8 Mon 17:30 BH-N 334

Growing drops on an inclined plate: Onset of sliding — •Simeon Völkel, Jonas Landgraf, and Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

Liquid drops sitting on or running down an inclined plane are ubiquitous in our daily lives. Their sliding can be triggered by tilting the surface at a fixed drop volume or by increasing the drop volume at a fixed inclination angle. Here, we present experiments on the latter protocol. Therefore we employ a conventional inkjet printhead, which provides a volume resolution of 23 picoliters, high repeatability, as well as the flexibility of following the drop's development by selecting different nozzles. Based on an analysis of both top view and side view images, we explore the evolution of the drop shape in the vicinity of the depinning transition and compare our results with numerical simulations.

CPP 18.9 Mon 17:45 BH-N 334

Contact angle saturation in electrowetting of nanodrops — •Nicolas Rivas and Jens Harting — Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11)

The wetting angle of a drop in contact with a substrate can be modified by applying an external electric field, a phenomenon referred to as electrowetting. The degree of wetting most commonly increases with the applied electric field, although in many cases only until a certain angle, after which the electric field has little or no influence on the wetting properties of the drop. This limit behavior is referred to as contact angle saturation (CAS). The origin of CAS is unknown, with numerous possible explanations present in the literature. In the following work we investigate electrowetting and CAS at the nanoscale. A model is proposed that takes into account the hydrodynamics of two fluids and the diffusion of charged solutes (ions). The numerical methodology used to solve this model is presented together with validation cases. The model is used to study electrowetting of conductive sessile drops as a function of the overall ion concentration and the relative conductivity of the two fluid phases. The variations of the contact angle are consistent with previous studies. We also observe CAS in regions of low salt concentration. A mechanism for CAS is proposed based on the progressive loss of ions from the drop as the electric field increases. This is discussed in relation to previously proposed mechanisms for CAS, which in general involve physics which our model does not intend to capture.

CPP 18.10 Mon 18:00 BH-N 334

Oblique Impact onto a Spherical Target — •Vignesh Thammanna Gurumurthy, Daniel Rettenmaier, Ilia V. Roisman, and Cameron Tropea — Insitute for Fluid Dynamics and Aerodynamics, Technical University of Darmstadt, Darmstadt,Germany

Drop impact onto spherical targets can be found in applications such as coating of particles in pharmaceutical products, spray encapsulation or agglomeration of particles in fluidized bed, etc. The chances of the drop impinging on the target asymmetrically are high which necessitates the understanding of its hydrodynamics. In this work, we investigate the drop impact onto spherical targets using numerical simulations. We use a modified version of volume of fluid method available in the open source code OpenFOAM for the simulations, with adaptive mesh refinement on the liquid-gas interface. Reynolds number and the off-axis distance between the target and the drop are the two parameters varied while the drop to target size ratio is kept constant. The impact is characterized by measuring the thickness of the film at the point of impact over time. Finally, an empirical correlation based on the Reynolds number for the residual film thickness will be presented.

CPP 18.11 Mon 18:15 BH-N 334

Morphological evolution of microscopic dewetting droplets with slip — Tak S. Chan[1], Joshua D. McGraw[1,2], Thomas Salez[3], Ralf Seemann[1], and •Martin Brinkmann[1] — [1]Experimental Physics, D-66123 Saarland University — [2]Département de Physique, Ecole Normale Supérieure/PSL Research University, CNRS, 24 rue Lhomond, 75005 Paris, France — [3]Laboratoire de Physico-Chimie Théorique, UMR CNRS Gulliver 7083, ESPCI Paris, PSL Research University, Paris, France

A liquid drop sitting on a smooth substrate will contract or spread depending on the equilibrium contact angle and the initial shape of the drop. One well known example is that of drops spreading over a completely wetting surface, which follow Tanner's law. In this study, we numerically compute the dynamics of contracting microscopic droplets where the slip-length b on the substrate is comparable to the intial drop height H. As quantified by the asphericity of the drop shape, we find a cross-over between two different dynamic regimes at slip length $b \ll H$ and $b \gg H$. These findings are explained from a competition between viscous dissipation in elongational flows for $b \gg H$, friction at the substrate for $b \approx H$, and viscous dissipation in shear flows for $b \ll H$. Following the changes between the dominant dissipation mechanisms, our study not only indicates two universal rescalings of the evolution of asphericity, but also a cross–over to the quasi-static shape evolution when b is many orders of magnitude smaller than the slip length b_m where the asphericity assume its maximum value.

CPP 18.12 Mon 18:30 BH-N 334

Role of hydrodynamics in chemically driven droplet division — •Rabea Seyboldt and Frank Jülicher — Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Macromolecular phase separation and droplet formation have long been proposed as key elements in the formation of protocells during the origin of life. A simple model of a protocell consists of a droplet, where droplet material is produced outside the droplet, and chemical reactions inside the droplet play the role of a simple metabolism. Our previous theoretical study showed that such chemically active droplets can have a flux-driven shape instability that leads to a symmetric droplet division. Here we study the role of hydrodynamic flows on the chemically driven droplet division. In the deformed droplet, gradients of Laplace pressure create the hydrodynamic flows that have a tendency to relax the droplet to a spherical shape. We find that despite these stabilizing flows, droplet division can still occur. We analyze the dependence of the instability on the droplet viscosity and parameters that characterize the metabolism and material production. A comparison with protein/RNA droplets suggests that the droplet division could be observable in experimental systems. This highlights the possibility that chemically driven shape instabilities could play a role for the organization of membrane-less organelles in biological cells. Additionally, our work provides a physical mechanism for the division of early protocells before the appearance of membranes.

CPP 18.13 Mon 18:45 BH-N 334

Content of secondary droplets formed by drop impact onto a solid wall wetted by another liquid — •Hannah M. Kittel, Ilia V. Roisman, and Cameron Tropea — Institute of Fluid Mechanics and Aerodynamic, Technische Universität Darmstadt, 64287 Darmstadt, Germany

Drop impact onto a wetted substrate is of importance in many engineering applications, for example in a combustion chamber, during spray coating or airframe icing.. The impact outcome s determined by the inertia, viscous and capillary forces. If the drop and wall film are of different fluids, the miscibility and the interfacial forces also influence the outcome. The composition of secondary drops resulting from such an impingement, and the state of the liquid film influence significantly the mixture preparation in either the engine or the catalytic converter. In the case of non-miscible fluids, the distribution of both fluids during and after the impact is important in order to understand the mechanism behind the drop impact of different liquids.

The main focus of this experimental work is on the impact of a single drop onto a thin, horizontal wall film of dif-ferent fluids. The liquids of drop and wall film are non-miscible in order to have a phase interface between both liquids. A dye is added to the liquid of the drop in order to distinguish both phases during and after the drop impact. The composition of the secondary droplets resulting from splashing, as well as the content of the partial rebound are characterized.

CPP 18.14 Mon 19:00 BH-N 334

Breakup of a stretching liquid bridge — •Sebastian Brulin, Ilia V. Roisman, and Cameron Tropea — Institute of Fluid Mechanics and Aerodynamics, Technische Universität Darmstadt, Darmstadt, Germany

Liquid bridge stretching occurs in many industrial applications like gravure printing, granulation of fine powders or fiber spinning. One industrial process where the phenomenon plays an important role is the ink transfer in gravure printing. This technique is used for the production of electrical circuits. The liquid is transferred from the printing role onto the printable substrate. During this transferring process the liquid forms a liquid bridge with the two substrates. In this work, the dynamics of a stretching liquid bridge between two solid plates, one of which moves with a constant acceleration, is studied using a high-speed video system. Experiments on fast bridge stretching and breakup were performed with the aim to measure the breakup time and the residual liquid volume at various initial gape thicknesses.

The measurements involve different non-dimensional initial gap heights (d= 0.1-0.4) for a wide range of accelerations (10 m/s2 -180 m/s2). The distilled water and water-gylcerol mixtures are used for the liquid bridge formation to investigate the effect of the viscosity and surface tension on the breakup time and breakup length. A semi-empirical model is developed in this study to predict these values.

CPP 19: Solid-liquid interfaces: Reactions and electrochemisty II (joint session O/CPP)

Time: Monday 16:45–18:15 Location: MA 144

CPP 19.1 Mon 16:45 MA 144

Pt modified Ru(0001) electrodes: structure-activity relationship for the CO and MeOH electrooxidation — •Albert K. Engstfeld, Jens Klein, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

Bimetallic PtRu catalysts are the most prominent catalyst material in polymer electrolyte membrane fuel cells for the electrooxidation of methanol (MeOH) since it enables the oxidation of the strong binding reaction intermediate CO from the surface at much lower overpotentials compared to a bare Pt catalyst. The underlying process is attributed to a so-called Langmuir Hinshelwood bifunctional mechanism, where the CO oxidation from Pt and Ru sites is promoted by the preferential adsorption of oxygen on neighboring Ru sites. In this work, we will show in comparison the electrocatalytic CO and MeOH oxidation on well defined Pt-modified Ru(0001) electrodes (surface alloys and Pt sub-/multilayer structures), prepared under UHV conditions and characterized on an atomic scale level with scanning tunneling microscopy (STM). For the surface alloys as well as submonolayer Pt-modified Ru(0001) we will show that the formation of bifunctional sites is indeed beneficial for the CO electrooxidation but is surprisingly inactive for the MeOH electrooxidation. On Pt multilayer structures, thus a surface without bifunctional sites, the MeOH electrooxidation is significantly more active compared to the mixed surfaces. Based on these results we will discuss the rate-limiting steps for the MeOH electrooxidation on these surfaces and discuss the influence of related electronic and geometric effects on both the CO and MeOH oxidation.

CPP 19.2 Mon 17:00 MA 144

Influence of Pt step sites on the electro-oxidation of CO — •Jens Klein, Valeria Chesnyak, Evelyn Artmann, Julian Bösking, Albert K. Engstfeld, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm

The performance of the CO electro-oxidation on Platinum (Pt) catalysts strongly depends on the surface structure of the catalyst. It has been reported that Pt electrodes with a large number of low coordinated step sites show an enhanced activity for the electro-oxidation of an adsorbed monolayer of CO, which was ascribed to active sites on the step edges.[1]

In this work we investigated the role of Pt steps in the electro-oxidation of CO on Pt electrodes under continuous CO supply (bulk CO oxidation). We prepared Pt(111) single crystal electrodes and varied the Pt step edge density by physical vapor deposition of Pt on the crystal under UHV conditions. The structural properties were characterized by scanning tunneling microscopy (STM). To identify the actual role of Pt step edges we blocked the respective sites, by decorating the Pt steps with a narrow Au film, since Au supported on Pt(111) was reported to be inert for the CO oxidation.[2] The electrocatalytic measurements, which were performed in an electrochemical flow cell, provide information on the role of the Pt steps in the CO oxidation and consequences of these findings will be discussed.

[1] G. García et al., ChemPhysChem. 12 (2011) 2064.

[2] D. C. Skelton et al., J. Phys. Chem. B, 103 (1999) 964.

CPP 19.3 Mon 17:15 MA 144

Comparing solvation effects on adsorbates at water/Pt(111) interface with implicit and explicit solvents — •Sung Sakong and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

For a realistic description of the elementary electrocatalytic processes at electrode/electrolyte interfaces, an adequate method to treat the solvated molecules at the interface is necessary. Since the solvation in liquid solvent requires thermodynamic sampling which is computationally demanding within ab initio molecular dynamics (AIMD) approach, numerically efficient implicit solvent methods which address solvation effects through a polarization potential and a corresponding electrostatic energy are becoming increasingly popular.

The structure of liquid water in the bulk and near electrode surfaces differs. Therefore we consider an implicit solvent method that determines cavitation on the fly using the charge density evaluated by quantum chemical methods. We will compare solvated reaction intermediates in the methanol electro-oxidation at the Pt(111)/water interface using an implicit solvent method and using explicit solvating water layer at the interface in order to assess the reliability of the implicit solvent approach.

[1] J. Chem. Phys. **142**, 234107 (2015).

[2] ACS Catal. **6**, 5575 (2016).

[3] Electrocatalysis **8**, 577 (2017).

CPP 19.4 Mon 17:30 MA 144

Microcalorimetric measurement of double layer charging in ionic liquids — •Jeannette Lindner[1], Fabian Weick[1], Stefan Frittmann[1], Frank Endres[2], and Rolf Schuster[1] — [1]Institute of Physical Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute of Electrochemistry, TU Clausthal, Clausthal, Germany

The reversible molar heats, i.e., the Peltier heats of processes in the electrified double layer at an IL/Au(111) interface were measured via electrochemical microcalorimetry. The Peltier heat corresponds to the entropy change during electrochemical double layer charging. 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide was used as ionic liquid. We found a decrease of ΔRS by 143 J/(K*mol) between E vs. Pt = -0,9 V and +1,0 V and ΔRS = 0 for E vs. Pt = -0,25 V. ΔRS = 0 corresponds to the maximum of the double layer formation entropy SMax. We interpret SMax as the maximum of mixing entropy of cations and anions within a lattice gas model with negligible ionic interactions. As a consequence, SMax corresponds to the pzc (point of zero charge) of the system. In order to quantitatively explain the found magnitude of the S variations, one has to include entropy contributions from multiple layers.

CPP 19.5 Mon 17:45 MA 144

A thermodynamic approach on specific anion adsorption via electrochemical Microcalorimetry — •Marco Schönig and Rolf Schuster — Karlsruhe Institute of Technology, Karlsruhe, Germany

The understanding of specific adsorption is of fundamental importance for the description of the electrochemical double-layer. With electrochemical microcalorimetry we measured the reversibly exchanged heat during the anion adsorption/desorption process, which is directly correlated with the reaction entropy of the electrochemical process (1). Using this method we investigated the adsorption of halides (Cl-, Br-, I-) and oxoanions (SO42-/HSO4-, CLO4-) on Au(111) as a function of the surface polarization. For all systems the exchanged heat increased in the adsorption region of the respective anion. A possible explanation may be the configuration entropy of an anion lattice gas.

(1) J. M. Gottfried und R. Schuster. Surface Microcalorimetry. In: Surface and Interface Science. Weinheim, Germany: Wiley-VCH Verlag GmbH & Co. KGaA, 2016, S. 73-126

CPP 19.6 Mon 18:00 MA 144

Enhanced Photoanode Activity with Co-Fe Prussian blue as genuine Water Oxidation Catalyst — •Franziska Hegner[1], Núria López[1], José-Ramón Galán Mascarós[1], and Sixto Gimenez[2] — [1]ICIQ Tarragona — [2]INAM, Castellón

Catalysts based on Prussian blue analogues have shown high water-oxidation efficiencies with exceeding long-term stabilities. Moreover, their application as co-catalysts on well-known photoanode materials, such as α-Fe2O3 and BiVO4, has shown success. We studied the electrochemical behaviour, catalytic efficiency and impedance under light and electrical field conditions. Also transient absorption spectroscopy (TAS) is used to gain more information about the behaviour of the system. In addition, we employed various theoretical simulations based on hybrid Density Functional Theory, DFT, and evaluated their applicability. With a combination of theoretical, as well as experimental studies, the true catalytic function of cobalt-iron Prussian blue as a co-catalyst on light-absorbing semiconductors can be evaluated.

CPP 20: Poster Session I

Topics: Bioinspired Functional Materials (20.1-20.4), Biomaterials and Biopolymers (20.5-20.12), Polymers in Multi-Compartment and Aqueous Solutions (20.13-20.21), Modeling and Simulation of Soft Matter (20.22-20.24), Data-driven Methods in Molecular Simulations of Soft-Matter Systems (20.25-20.26), Polymer Networks and Elastomers (20.27-20.29), Polymer and Molecular Dynamics (20.30-20.33), Molecularly Functionalized Low-Dimensional Systems (20.34-20.35), Charged Soft Matter, Polyelectrolytes and Ionic Liquids (20.36-20.47), Crystallization, Nucleation and Self-Assembly (20.48), Interfaces and Thin Films (20.49-20.62).

Time: Monday 17:30–19:30 Location: Poster A

CPP 20.1 Mon 17:30 Poster A

Dry adhesives of structured polydimethylsiloxane — •Andreas Zheng[1], Volker Körstgens[1], Hsin-Yin Chiang[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Rythm, 75009 Paris, France

Biocompatible, gecko-inspired dry adhesives are fabricated using polydimethylsiloxane (PDMS) in a 2-step fabrication process. First uncured PDMS is filled into a silicon mold of a regular hole pattern. After degassing and curing a PDMS replica containing a regular pillar pattern is obtained. In the second step the pillars of the PDMS replica are dipped into a thin film of liquid PDMS and attached onto an anti-adhesive film to achieve a mushroom-tip structure upon curing. The dimensions and the geometrical shapes of the achieved structures are investigated with optical microscopy. Adhesive forces of the PDMS patches in contact with different materials are measured with a tack test. Force-distance curves are obtained using a home-built instrument with a unique punch design developed for pressure sensitive adhesives. The dependence of adhesion forces on the structure of the PDMS patches is presented.

CPP 20.2 Mon 17:30 Poster A

Imitation of scattering networks by foam models — •Dominic Meiers[1], Marie-Christin Angermann[1], and Georg von Freymann[1,2] — [1]Physics Department and Research Center OPTIMAS, University of Kaiserslautern, Kaiserslautern, Germany — [2]Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, Germany

The wing scales of the beetle Cyphochilus show one of the highest whiteness and brightness found in nature, although they are only about 5 μm thick [1]. This brilliant whiteness is achieved by multiple light scattering in the inner disordered chitin network of the scales [2]. To model and optimize this network, a foam model generator (GeoDict) is used. This foam has an inner structure comparable to the beetle's network. By varying the parameters of generation, the optical properties are optimized in respect of whiteness and brightness. Therefore, the optical response is calculated by using a finite difference time domain method. Moreover, the foam structure is compared with the measurement-based model of the chitin network shown in [3]. Subsequent steps are the further improvement of the foam structure and its fabrication via 3D direct laser writing. Eventually, it might be possible to create artificial structures that are comparable to the beetle's wing scales in the near future.

[1] P. Vukusic, B. Hallam, J. Noyes, Science 315, 5810 (2007). [2] M. Burresi et al., Scientific Reports 4, 6075 (2014). [3] B. Wilts et al., Adv. Mater. 2017, 1702057 (2017).

CPP 20.3 Mon 17:30 Poster A

Entangled Nets from Surface Drawings — •Benedikt Kolbe — Institute of Mathematics, Technische Universität Berlin

Imagine drawing a few lines on an arbitrary surface. What if the drawing for the rest of the surface can be filled in by invoking symmetries? Is there a way to enumerate different ways of scribbling? If the goal was to find molecular structures by drawing them on surfaces, what surfaces would we start with and why?

This talk will motivate and answer these questions, while focusing on a new technique to explicitly enumerate and construct all essentially different ways to decorate prominent examples of triply periodic minimal surfaces with a given symmetry. We will also touch upon what kind of 3D structures arise in this way.

There will be tie-ins to geometry, braid theory, combinatorial group and tiling theory, physics, and even some chemistry.

CPP 20.4 Mon 17:30 Poster A

Rearrangement of nanopatterns: Wetting of n-alkane Molecular Films — Diego Diaz[1], Tomas P. Corrales[2], Maria J. Retamal[3], Marcelo Cisternas[1], Nicolas Moraga[1], Rodrigo Catalan[1], Mark Busch[4], Patrick Huber[4], Marco Soto-Arriaza[3], and •Ulrich G. Volkmann[1] — [1]Institute of Physics and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — [2]Department of Physics, UTFSM, Valparaiso, Chile — [3]Faculty of Chemistry and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — [4]TUHH, Hamburg, Germany

We present a study of the wetting properties of silicon samples coated with a single layer of n-alkane molecules self-assembled perpendicular to the surface. It is known that the filling fraction (between 10% to 50%) of molecules on the surface can be controlled by the withdrawal velocity of the silicon wafer from the coating solution. After sample preparation, the contact angle was measured of a 2 microliter drop of water placed on the patterned surface. The results of the apparent contact angle versus coverage can be grouped in two regimes that depend linearly on coverage, which is consistent with the Cassie wetting model. After drop evaporation, the molecules migrate to the center and the contact line of the area where the sessile drop was placed, leaving also a depletion zone. AFM studies showed that the original patterns restructure. Acknowledgements: Postdoctoral FONDECYT #3160803 (MJR), FONDECYT #1141105 (UGV) and #1171047 (MSA), FONDECYT INICIACION #11160664 (TPC), CONICYT Fellowships (RC, MC) and CONICYT-PIA ACT 1409.

CPP 20.5 Mon 17:30 Poster A

Microrheology of hydrogel-like biological materials — •Elke Bradt[1], Sabine Hild[1], Erwin K. Reichel[2], Thomas Voglhuber-Brunnmaier[2], and Milan Kracalik[1] — [1]Johannes Kepler University, Institute of Polymerscience, Linz, Austria — [2]Linz Institute of Technology, Institute for Microelectronics and Microsensors, Linz, Austria

Rheology of biofluids introduces a new inside into medical technology and is crucial for the associated physiological function. Typical example for biofluids is synovial liquid, which can be found in joints. The viscosity and elasticity of synovial fluids are essentially determining the ability to maintain the joint spacing, reduce slip resistance, and protect cartilage from abrasion. Biological elastic liquids show pronounced extensional viscosity, they are therefore often analyzed using capillary breakup rheometry. Comparing to this method microrheological investigation e.g. passive microrheology based on dynamic light scattering is in the meantime a common technique using commercial equipment. In order to be conform with actual ethics in medicine research, for preliminary studies (optimization of measuring conditions like tracer selection, temperature, pH) model liquids are important. In this work different model liquids, which are physiologically similar to synovial liquid, have been explored and measured using passive microrheology. The differences in viscoelastic behavior between model liquids and synovial liquid were evaluated.

CPP 20.6 Mon 17:30 Poster A

Protein exchange on Gold Nanoparticles – Tailored Polymers as model systems — •Carmen Radeke[1,2], Jonas Schubert[1,3], Munish Chanana[4,5], and Andreas Fery[1,3] — [1]Department of Nanostructured Materials, Leibniz-Institut für Polymerforschung Dresden e. V. — [2]Department of Biopolymers, University of Bayreuth, 95440 Bayreuth, Germany — [3]Physical Chemistry of Polymer Materials, Technische Universität Dresden, D-01062 Dresden, Germany — [4]Institute of Building Materials (IfB), ETH Zurich, 8093 Zurich, Switzerland — [5]EMPA Dübendorf, 8600, Dübendorf, Switzerland.

Understanding the behavior of NPs in biological systems is one of the major challenges on the way to new therapeutics and diagnosis tools in medicine. Therein, the generation of an undefined protein corona is a crucial point, as by this, the physicochemical properties of the NPs and therefore also their behavior change drastically. To address these problems, we used a defined protein corona on Au NP as model system. This has the advantage that a fluorescent labeled protein shell can be detected when being exchanged. To understand the influence of physicochemical parameters (e.g. molecular weight, functional groups and concentration of free protein) of protein exchange under physiological conditions, we simplified the system by using polymer and polypeptides as model systems.

CPP 20.7 Mon 17:30 Poster A

Adsorption of finite semiflexible polymers and their loop and tail distributions — •Tobias A. Kampmann and Jan Kierfeld — TU Dortmund University, Germany

We discuss the adsorption of semiflexible polymers to a planar attractive wall and focus on the questions of the adsorption threshold for polymers of finite length and their loop and tail distributions using both Monte-Carlo simulations and analytical arguments. For the adsorption threshold, we find three regimes: (i) a flexible or Gaussian regime if the persistence length is smaller than the adsorption potential range, (ii) a semiflexible regime if the persistence length is larger than the potential range, and (iii) for finite polymers, a novel crossover to a rigid rod regime if the deflection length exceeds the contour length. In the flexible and semiflexible regime, finite size corrections arise because the correlation length exceeds the contour length. In the rigid rod regime, however, it is essential how the global orientational or translational degrees of freedom are restricted by grafting or confinement. For the loop and tail distributions, we find power laws with an exponential decay on length scales exceeding the correlation length. This allows us to explain that, close to the transition, flexible and semiflexible polymers desorb by expanding their tail length.

CPP 20.8 Mon 17:30 Poster A

Non-Classical Interactions of Phosphatidylcholine with Mucin for Protection of Intestinal Surfaces: A Microinterferometry Study — •Federico Amadei and Motomu Tanaka — Institute of Physical Chemistry, Heidelberg, Germany

Albeit many studies demonstrated that the accumulation of phospholipids in the intestinal mucosal surfaces is essential for the protection of colon epithelia against pathogenic bacteria, the mechanism of interactions between phospholipids and the surface protein mucin is not well understood. In this study, the significance of phospholipid-mucin interactions was quantified by the combination of an in vitro intestinal surface model and label-free microinterferometry. The model of intestinal surfaces consists of planar lipid membranes deposited on solid substrates that display mucin proteins at defined anchoring densities. Following the characterization of the systems by quartz crystal microbalance and fluorescence staining, the vertical Brownian motion of cell-sized particles on model surfaces was monitored by using RICM. In case of latex particles bearing different surface charges, the calculated potential curvature monotonically increased according to the increase in surface potential, suggesting the dominant role of electrostatic interactions with negatively charged mucin in the potential confinement. However, the particles coated with phospholipids exhibited a clear nonlinearity: the particles coated with zwitter-ionic phosphatidylcholine is most sharply confined on mucin surfaces. Our data suggested the presence of another underlying molecular level interaction that is stronger than electrostatic interactions.

CPP 20.9 Mon 17:30 Poster A

In situ GISAXS analysis of spray deposited metal-biopolymer thin films — •Wiebke Ohm[1], Michał Kamiński[1], Pallavi Pandit[1], Calvin Brett[1,2], Shun Yu[2], Nitesh Mittal[2], Daniel Söderberg[2], and Stephan V. Roth[1,2] — [1]Deutsches Elektronen-Synchrotron Hamburg, Notkestraße 85, 22607 Hamburg — [2]KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, Teknikringen 56-58, SE-100 44 Stockholm, Sweden

Conductive polymer substrates based on metal coated cellulose layers offer a renewable and sustainable replacement for synthetic polymer substrates, which is essential for many applications in nanotechnology. In order to reach this target, we follow a route combining cellulose nanofibril thin films with silver nanowire (Ag NW) coating offering the additional advantage of transparency. For effective industrial fabrication, not only the controlled arrangement of the precursors during the deposition process is essential but also the use of an industrial compatible deposition process. Air-brush spray deposition is a versatile deposition technique that fulfils industrial demands and was thus chosen for preparation of metal-cellulose thin films.

We investigated all spray deposited cellulose/Ag NW layer form aqueous and alcoholic solution. In situ grazing incidence small angle x-ray scattering (GISAXS) in combination with microscopy techniques of the final layers revealed the inner structure and arrangement of these films. The conductivity and transparency as function of surface coverage are investigated for Ag NW deposited on different substrates. First GISAXS results of aligned Ag NW will be presented.

CPP 20.10 Mon 17:30 Poster A

Raman spectroscopy on bioinorganic model complexes — •Dieter Rukser[1], Florian Biebl[1], Melissa Teubner[1,2], Benjamin Grimm-Lebsanft[1], Patricia Liebhäuser[2], Sarah Neville[3], Alexander Hoffmann[2], Linda Doerrer[3], Sonja Herres-Pawlis[2], and Michael Rübhausen[1] — [1]Center for Free Electron Laser Science, Universität Hamburg — [2]Instiut für anorganische Chemie, RWTH Aachen — [3]Inorganic Chemistry, Boston University

Elucidating charge-transfer dynamics of transition metal complexes is crucial for the understanding of a multitude of biochemical processes. Raman spectroscopy is a useful tool to study model complexes mimicking these processes.

By resonant excitation of the transition state, the electron transfer is accessible through vibrational modes, which are coupled to metal-ligand charge transfer (MLCT) and ligand-metal charge transfer (LMCT) states.

We have studied bioinorganic copper complexes using resonant as well as time-resolved Raman spectroscopy. For complexes stable at temperatures below -60 °C we have designed a Peltier cooled cryostat for our UT-3 Raman spectrometer, allowing operando oxygenation and measurement of the samples at temperatures down to -90 °C.

For samples that are damaged by laser radiation, we have designed several jet-based delivery systems. Jet diameters down to 10 μm and flow rates of 15 μL/min allowed us to measure small sample volumes for several hours.

CPP 20.11 Mon 17:30 Poster A

Simulations of linear and cyclic RGD peptides at a free surface of the polymer brushes — •Olga Guskova[1,2], Ulla König[1], Petra Uhlmann[1], and Jens-Uwe Sommer[1,2] — [1]IPF Dresden — [2]DCMS, TU Dresden

Motivated by recent experiments [1,2] aiming at biomimetic design of new polymeric surfaces relevant for the biotechnological applications, the behaviour of short peptides with the RGD motif, mimicking the cell adhesion proteins, is simulated using DFT/MD combination. Three peptides are modeled: linear GRGDS, linear GRGDSPK and cyclic cRGDyK in aqueous solutions and being chemically attached to the PAA brush surface. For free peptides, the net charge and the charge pattern are characterized and the most reactive amino-groups are predicted based on the ESP charges. The free energy of hydration calculated by thermodynamic integration shows the negative values and changes in the row GRGDS>GRGDSPK>cRGDyK. Secondary structures of linear peptides have "normally allowed" β-regions, β-turns and coil-like structures, whereas the cyclic chain is sterically restraint. The secondary structures and the radial distribution functions of water around the charged peptide groups are calculated for the chains attached to PAA backbone. We compare the shielding and exposure of bound GRGDS, GRGDSPK and cRGDyK peptides and the availability of the RGD sequence and R-side chain at the brush surface.

[1] E. Psarra et al. ACS Omega, 2017, 2, 946.

[2] U. König et al. Biointerphases 2017 (submitted).

CPP 20.12 Mon 17:30 Poster A

A Theoretical Study of the Interaction of Calcite with Amino Acids — •Robert Stepić[1,2], Zlatko Brkljača[1,2,3], Ana-Sunčana Smith[1,2,3], and David M. Smith[2,3] — [1]FAU, Institute for Theoretical Physics I, PULS Group, Erlangen, Germany — [2]Cluster of Exellence: Engineering of Advanced Materials, Erlangen, Germany — [3]Rudjer Bošković Institute, Zagreb, Croatia

Calcite is one of the most widespread minerals on earth which interacts favourably with a variety of biomolecules. This interaction can mediate the growth of calcite resulting in formation of biominerals with remarkable mechanical properties useful in a number of applications. In this work we utilize a bottom-up approach and study the interaction of protein building blocks, amino acids, with the stable (104) surface of calcite. We also probe the interactions with different morphologies deriving from (104) surface which incorporate kinks and edges. Amino acids are studied in their native zwitterionic and protected forms. Our method of choice for this study encompasses fully atomistic molecular dynamics simulations using state of the art force fields for these types of systems. We employ enhanced sampling techniques with biasing potentials to obtain free energy profiles along the axis perpendicular to the surface. This enables us to estimate the free energies of binding of amino acids to the calcite and also gives us the information on the molecular details of the interaction. These results provide a force field benchmark and reference data on binding energies of specific amino acids which could help interpret the experimental data on peptide and protein mediated calcite functionalization and growth.

CPP 20.13 Mon 17:30 Poster A

SANS Study on the Pressure-Dependence of the Cononsolvency Effect in Aqueous PNIPAM Solutions — •Bart-Jan Niebuur[1], Kora-Lee Claude[1], Ralf Schweins[2], Vitaliy Pipich[3], Marie-Sousai Appavou[3], Alfons Schulte[4], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Institut Laue-Langevin, Grenoble, France — [3]JCNS at MLZ, FZ Jülich, Garching, Germany — [4]University of Central Florida, Department of Physics, Orlando, U.S.A.

The solubility of the thermoresponsive polymer poly(N-isopropylacrylamide) (PNIPAM) in aqueous solutions decreases drastically when small amounts of methanol are added, resulting in a reduced cloud point, an effect called cononsolvency. If high pressure is applied, the cononsolvency effect is destroyed, meaning that the cloud point is clearly higher in comparison with PNIPAM solutions in pure water at the same pressure. Using small-angle neutron scattering, the phase behavior of semi-dilute PNIPAM solutions in mixtures of water and methanol is studied in temperature scans at various pressures, revealing the behavior of the concentration fluctuations near the respective cloud points. The results show that high pressure strongly broadens the phase transition, revealing changes in the polymer-solvent interaction. Very small-angle neutron scattering allowed us to study the effect of methanol on the mesoglobule formation and the size of the mesoglobules in the segregated state of PNIPAM at high pressure.

CPP 20.14 Mon 17:30 Poster A

The structural, thermal and dynamic behavior of the thermoresponsive polymer Poly(N-isopropylmethyacrylamide) — •Chia-Hsin Ko[1], Kora-Lee Claude[1], Dirk Schanzenbach[2], Bart-Jan Niebuur[1], Xiaohan Zhang[1], Dionysia Aravopoulou[3], Apostolos Kyritsis[3], Henrich Frielinghaus[4], Peter Müller-Buschbaum[1], André Laschewsky[2,5], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Universität Potsdam, Institut für Chemie, Potsdam-Golm, Germany — [3]National Technical University of Athens, Greece — [4]Forschungszentrum Jülich GmbH, JCNS at MLZ, Garching, Germany — [5]Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm, Germany

Poly(N-isopropylmethyacrylamide) (PNIPMAM) is a thermoresponsive polymer, exhibiting lower critical solution temperature (LCST) behavior in aqueous solution with a cloud point at ~43 °C. We investigate the temperature- and concentration-dependent phase behavior of PNIPMAM in D2O using turbidimetry, differential scanning calorimetry (DSC), small-angle neutron scattering and dynamic light scattering. We find that the phase transition consists of two steps, namely (i) hydrophobic aggregation at ~39 °C, as evident from turbidmetry and SANS and (ii) the chain collapse and water release at ~44 °C, as evident from DSC and SANS.

CPP 20.15 Mon 17:30 Poster A

Thermodynamics of polyNIPAM – simulation study — •Vladimir Palivec, Denis Zadrazil, and Jan Heyda — University of Chemistry and Technology, Prague, Czech Republic

Among thermoresponsive polymers, Poly-N-isopropyl acrylamide (PNIPAM), plays a prominent role, both in simulations, theory, and in applications. Nevertheless, the microscopic description of a PNIPAM chain collapse transition above the LCST is still puzzling and challenges the computational chemists for last decades. In this contribution, we have employed large-scale atomistic computer simulations of single PNIPAM chain in explicit water. We have analyzed swollen-to-collapse transition thermodynamics and the values were compared with in house performed experimental data, such as calorimetric or volumetric.

CPP 20.16 Mon 17:30 Poster A

NiPAM-salt interactions in aqueous solutions — •Jakub Polák, Vladimír Palivec, Adam Kovalčík, Pavel Vrbka, Daniel Ondo, and Jan Heyda — Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech Republic

This contribution is focused on a physico-chemical characterization of N-isopropyl-acrylamide (NiPAM) in aqueous solutions of sodium and guanidinium salts. To describe the NiPAM-salt interaction, two properties were chosen. The preferential binding of salt over that of water to the NiPAM surface, which was determined by vapor pressure osmometry (VPO), and the partial molar volume of NiPAM in salt solutions determined from large set of density measurements.

Firstly acquired data for preferential binding were used to evaluate the Salting out (Setschenow) constants and compared to literature values for similar amides. Secondly the relevant Kirkwood-Buff integrals were calculated, by joining data from osmometric and densimetric measurements. Last, the thermodynamic properties of NiPAM were compared with data for thermoresponsive polymer polyNiPAM obtained from our recently derived thermodynamic model and its combination with the Kirkwood-Buff theory of solutions.

CPP 20.17 Mon 17:30 Poster A

Morphology of Amphiphilic Bottlebrush Copolymers in Dilute Aqueous Solution — •Jia-Jhen Kang[1], Kaltrina Shehu[1], Junpeng Zhao[2], Stergios Pispas[2], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece

Densely grafted copolymers, or polymeric bottle brushes, present a complex architecture. We investigate polymeric bottle brushes having diblock or random copolymers as side arms. These comprise poly(ethylene oxide) and poly(propylene oxide), where the former is water-soluble and the latter becomes hydrophobic at elevated temperatures, which leads to increased turbidity both for diblock and for random side arms [1]. In the present study, we aim to characterize their temperature-dependent conformation and self-assembly in dilute aqueous solution using dynamic light scattering and small-angle X-ray scattering. Comparing the data of the bottle brushes with analogous linear polymers, we gain insight into the effects caused by the complex architecture.

[1] J. Zhao et al., J. Polym. Sci.: Part A: Polym. Chem. 48, 2320 (2010) and Macromolecules 43, 1771 (2010).

CPP 20.18 Mon 17:30 Poster A

Morphological study of drug delivery systems based on poly(2-oxazoline) bottle brushes — •Kaltrina Shehu[1], Jia-Jhen Kang[1], Clemens Sachse[2], Rainer Jordan[2], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]TU Dresden, Professur für Makromolekulare Chemie, Dresden, Germany

Nano carriers for drug delivery have traditionally been based on the self-assembly of amphiphilic block copolymers. These typically form spherical micelles which can incorporate hydrophobic drugs. It has been shown, however, that it is an advantage if the polymeric nanoparticles are elongated. Densely grafted copolymers, or polymeric bottle brushes, form unimolecular elongated nanoparticles. If their side arms are amphiphilic, they may incorporate hydrophobic drugs. Poly(2-oxazoline)s are highly biocompatible and may be rendered hydrophilic or hydrophobic by the choice of the side group, and are thus of interest for this application. Here, we investigate the concentration and temperature-dependent size, shape and inner structure of a polymeric bottle brush, having a poly(2-isopropenyl-2-oxazoline) backbone and poly(2-ethyl-2-oxazoline) side chain in dilute aqueous solution using dynamic light scattering (DLS) and small angle X-ray scattering (SAXS).

CPP 20.19 Mon 17:30 Poster A

A wide range of surface forces of PSS terminated polyelectrolyte multilayers — •Heba Soker Mohamad, Sven Neuber, Annkatrin Sill, and Chistiane A. Helm — Institut für Physik, Uni. Greifswald, Felix-Hausdorff-Str. 6 17489 Greifswald

Films built from the Poly (styrenesulfonate) (PSS) and poly (diallylmethylammonium) (PDADMA) in 0.1 Mol/L NaCl are investigated. Film build-up starts with a parabolic growth regime, followed by a linear growth regime. In the former positive PDADMA and negative PSS monomers are balanced; in the latter an excess of PDADMA monomers is balanced by Cl- ions. Colloidal probe measurements show that in the former PSS-terminated films are flat and negative, in the latter they are electrically neutral at 0.1 Mol/L NaCl and are positively charged at other ion concentrations . If exceeds 1 Mol/L steric forces are found. Thus, by choosing the growth regime and suitable post-preparation treatment the surface forces can be tuned.

CPP 20.20 Mon 17:30 Poster A

Scattering Behavior of Distorted Semi-Flexible Polymers and Semi-Flexible Random Copolymers — •Reinhard Sigel — Max-Planck-Institut für Eisenforschung, Düsseldorf

Models for the interpretation of scattering experiments for two classes of polymer systems are discussed. In distorted semi-flexible polymers, the orientation correlation of the chain gets lost at distortions (kinks). A statistical combination of different monomers results in a random copolymer, where the orientation correlation is affected by the persistence lengths of the respective homo-polymers. In a dilute solution condition, the description of both polymer systems can be traced back to suitable averages of form factors from the literature. To handle the contrast difference in random copolymers, the approach of Endo and Shibayama (Polymer J. 42, 157-160, 2010) for flexible chains is extended to the case of semi-flexible chains.

CPP 20.21 Mon 17:30 Poster A

One-Pot Synthesis of Copper Oxide Nanowires and PVDF/CuO Composite Films for Piezoelectric Energy Harvesting Application — Samiran Garain[1], •Karsten Henkel[1], Dipankar Mandal[2], and Dieter Schmeisser[1] — [1]Angewandte Physik-Sensorik, Brandenburgische Technische Universität Cottbus-Senftenberg, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]Organic Nano Piezoelectric Devices Laboratory, Jadavpur University, Kolkata-700032, India

Copper oxide (CuO) is an attractive p-type oxide semiconductor with narrow band gap that has intriguing properties such as non-toxicity, chemical stability, electrocatalytic activity, abundant availability and low production cost. Polymeric materials have attracted great interest owing to their high flexibility, light weight, low cost production and high resistance against corrosion. Poly(vinylidene fluoride) (PVDF) is a commonly used piezoelectric polymer due to its excellent flexibility and piezoelectric properties. In this work, we adopted a one-pot synthesis of CuO nanowires by facile and selective chemical etching process of Cu substrate. XPS, XRD, SEM data ascribed the formation of polycrystalline CuO nanowires over the entire Cu surface. It has been observed that the uniformity, shape and size of the nanowires could be conveniently controlled by etching time and etchant concentration. We have also prepared piezoelectric nanogenerator based on the flexible PVDF/CuO composite film, where the traditional electrical poling treatment was avoided. In addition, dielectric properties have been studied to demonstrate the role of interfacial polarization.

CPP 20.22 Mon 17:30 Poster A

Molecular dynamics simulation of hyperbranched polymers as a twofold distributed polymer system — •Peter Friedel[1], Shamila Firdaus[1,2], Albena Lederer[1,2], and Susanne Boye[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany

The properties of hyperbranched polymers are determined by a molar mass and a configuration distribution which makes the experimental characterization difficult.

The developement of a simple simulation approach which may describe the properties of such a twofold distributed hyperbranched polymer system is the aim of the following denoted procedure. Starting with a well optimized monomer unit one may build up a set of hyperbranched polymer models (e.g., the specific poly(2,2-bis(hydroxymethyl)propionic acid) polymer system) with different molar masses and configurations (from linear over hyperbranched up to dendritic ones). Performing corresponding molecular dynamics simulations of every model of this set diluting it in an explicit solvent (i.e. THF) and equilibrating the whole NpT ensemble up to a standard state one is able to evaluate the corresponding trajectories (time averaged radii of gyration, monomer densities, pair distance distributions etc.).

These results may be weighted summarized and represent the properties of the called polymer system which are comparable to the experimental findings and to corresponding MC simulations (NVT ensemble with implicit solvent).

CPP 20.23 Mon 17:30 Poster A

Event-chain simulations of many semiflexible polymers — •Tobias A. Kampmann and Jan Kierfeld — TU Dortmund University, Germany

We applied the extended, parallel EC algorithm to a system of many (semiflexible) harmonic chains, where the simulation efficiency is comparable to optimized molecular dynamics simulations, while still incorporating the essential features of the actual dynamics. This novel algorithm allows the simulation of melts of hard needle polymers - chains of infinitely thin rods - where reptational behaviour can be clearly observed. When the polymers interact via a short range, attractive square well potential bundled structures arise. It is not known, neither experimentally nor theoretically, what the actual thermodynamic equilibrium state of such a system is and whether this state can be achieved kinetically at all, depending on the initial conditions. Possible equilibrium structures are a single thick bundle or networks of smaller bundles. In any case, tightly packed bundles are created, which are difficult to equilibrate with traditional local moves. The use of EC algorithms thus appears to be advantageous.

CPP 20.24 Mon 17:30 Poster A

Assignment of polymer geometries in STM images via statistical analysis of fitted patterns — •Florian Günther[1,2,3], Dmitry Skidin[1,3], Francesca Moresco[1,3], Gianaurelio Cuniberti[1,3], Sibylle Gemming[2,3,4], and Gotthard Seifert[1,3] — [1]TU Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [3]Center for Advancing Electronics Dresden, Germany — [4]TU Chemitz, Germany

To study the physical properties of a system on the atomic scale, the geometry is an important issue. For soft materials, however, the geometry is a priori unknown and hard to access experimentally.

In this work, we study the donor-acceptor polymer poly-dithienyl-diketopyrrolopyrrole (pTDPP) for which we analysed the impact of the torsion angles on the stability of the system. For this, we used density functional theory (DFT) methods using different functionals as well as the computationally efficient density functional based tight binding (DFTB) approach.

Moreover, we consider scanning tunnel microscopy (STM) images of pTDPP obtained via on-surface polymerization at Au(111). Here, we use an empirical fitting of frequently occurring patterns and analyse the obtained distances and angles statistically. In doing so, we could clearly assign certain geometries of the polymer found by simulation to the STM patterns.

CPP 20.25 Mon 17:30 Poster A

Machine learning of correlated dihedral potentials for atomistic molecular force fields — •Pascal Friederich[1], Manuel Konrad[1], Timo Strunk[2], and Wolfgang Wenzel[1] — [1]Karlsruhe Institute of Technology, Karlrsuhe, Deutschland — [2]Nanomatch GmbH, Karlsruhe, Deutschland

Computer simulation increasingly complements experimental efforts to describe nanoscale structure formation. Molecular mechanics simulations and related computational methods fundamentally rely on the accuracy of classical atomistic force fields for the evaluation of inter- and intramolecular energies. One indispensable component of such force fields, in particular for large organic molecules, is the accuracy of molecule-specific dihedral potentials which are the key determinants of molecular flexibility. We show in this work that non-local correlations of dihedral potentials play a decisive role in the description of the total molecular energy - an effect which is neglected in most state-of-the-art dihedral force fields. We furthermore present an efficient machine learning approach to compute intramolecular conformational energies. At the example of α-NPD, a prototypical molecule used in organic electronics, we demonstrate that this approach improves the agreement between semi-empirical energies and traditional force fields by one order of magnitude to a mean absolute deviation smaller than 0.37 kcal/mol (16.0 meV) per dihedral angle.

CPP 20.26 Mon 17:30 Poster A

Quantifying how coarse-graining reduces the size of chemical compound space — •Kiran Kanekal, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research

Increasing the efficiency of materials design and discovery remains a significant challenge, especially given the prohibitively large size of chemical compound space. Efficient sampling of chemical compound space can be achieved *in silico* with the use of transferable coarse-grained (CG) models that retain the essential properties of a higher resolution method. In addition to reducing computational expense, use of a chemically transferable CG model enables different molecular fragments to map to the same bead type. This further increases sampling efficiency, effectively reducing the size of chemical compound space. For example, the MARTINI[1] force field consists of 14 different neutral bead types, allowing for 119 unique representations consisting of 1-bead and 2-bead CG molecules. We previously showed that over 400,000 molecules could be mapped to these 119 MARTINI representations, demonstrating a drastic reduction of chemical compound space[2]. However, it is unclear as to how much variability exists within the subset of molecules and functional groups that map to a single bead type. In this work, we investigate these subsets for each MARTINI bead type to quantify the effective range of chemical space that is covered by that bead type. We further propose new criteria for the rational design of CG models that allows for the optimization of their chemical transferability. [1] Fink and Reymond, J. Chem. Inf. Model. 2007, 47, 342. [2] Menichetti et al., J. Chem. Phys. 2017, 147, 125101.

CPP 20.27 Mon 17:30 Poster A

The elasticity of real polymer networks without entanglements — •Michael Lang[1], Toni Müller[1,2], and Jens-Uwe Sommer[1,2] — [1]Institut Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany — [2]Technische Universität Dresden, Institut für Theoretische Physik, Zellescher Weg 17, 01069 Dresden, Germany

We develop a method that allows to analyze directly the local contributions of individual strands to rubber elasticity. This method is used to quantify the impact of cyclic defects on elasticity for 4-functional model networks that were prepared at a different polymer volume fraction and with a different degree of polymerization between the crosslinks. Using the bond fluctuation model for simulations, entanglements and excluded volume can be switched off separately, which allows for a direct quantification of the effect of excluded volume on the phantom modulus of a network. We test our estimate of the phantom modulus with the modulus as measured from shearing the networks without excluded volume. For networks with excluded volume switched on, we find that excluded volume renormalizes fluctuations but has virtually no impact on the elasticity of the networks. However, the inactive material, which is connected to the network through a single point now couples partially to the shear deformation of the elastically active network, such that considering a zero contribution of the inactive material underestimates the phantom modulus.

CPP 20.28 Mon 17:30 Poster A

Development of a self-healing silicone rubber for high-voltage cable accessories — •Lena Barnefske[1], Andreas Petersen[2], Gerd Heidmann[2], and Heinz Sturm[1] — [1]Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany — [2]Institut Prüffeld für elektrische Hochleistungstechnik GmbH, Berlin, Germany

Self-healing materials are modified materials which respond on a damage phenomenon by using a damage management, called self-healing. In the scope of this research it is important that such materials are developed for a specific damage phenomenon as well as on a specific application. One of the biggest problems in high-voltage silicone rubber insulation cable accessories is the damage on electrical treeing, initiated by partial discharges. This damage leads at one point to a breakdown of the insulation. Furthermore, these cable accessories are often difficult to access. This aspects open up a question whether novel and promising self-healing materials might be a solution to this problem.

Our research focuses on a highly homogeneous material design, which is composed by a silicone rubber matrix with polydimethylsiloxane-polyorganosilioxane filler particles. Particles are able to release polydimethylsiloxane after destruction for healing. With our contribution we would like to present first results on the characterization on the damage mode induced by electrical treeing under high-voltage with scanning electron microscopy to define parameters for further developments on the material.

CPP 20.29 Mon 17:30 Poster A

Intercalation of p-aminobenzoic acid into layered cobalt hydroxide salt using a hydrothermal methodology: synthesis, characterization, and evaluation as potential modifier of polyethylene of absorption ultraviolet ray properties — •neffer gomez[1], swami maruyama[1], fernando wypych[1], and andreas leuteritz[2] — [1]Universidade Federal do Parana,curitiba, brazil — [2]leibniz institutes für polymerforschung

This paper aims to synthesize nanocomposites based in hydroxide salts intercalated with organic ultraviolet (UV) absorbent molecule for use in the lining of cables that could be apply in the electrical center. The synthesis procedure was performed using urea hydrolysis of Co (II) nitrate melts at 160 °C and its modification carry-out in an oven at 90 and 120 °C in a simple process. The modified structure and thermal stability of the hydroxide salt with formula (Co(OH)1,7(PABA)0,3).0,443H2O were characterized by XRD, FTIR, TGA, Raman, DSC, UV-Vis, MEV. Its studies suggest that HNCo-AB may have potential application as a UV absorber, because it improves this property when mixing with polyethylene,when the UV spectra shows a big band that covered the region between 400-200 nm.

CPP 20.30 Mon 17:30 Poster A

Molecular Modeling of Polycarbonate Materials: Glass Transition and Mechanical Properties — •Karol Palczynski[1], Andreas Wilke[2], Manfred Paeschke[2], and Joachim Dzubiella[1] — [1]Institut für Weiche Materie und Funktionale Materialien, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner Platz 1, 14109 Berlin, Germany — [2]Bundesdruckerei GmbH, Kommandantenstraße 18, 10969 Berlin, Germany

Linking the experimentally accessible macroscopic properties of thermoplastic polymers to their microscopic static and dynamic properties is a key requirement for targeted material design. Classical molecular dynamics simulations enable us to study the structural and dynamic behavior of molecules on microscopic scales, and statistical physics provides a framework for relating these properties to the macroscopic properties. We take a first step towards creating an automated workflow for the theoretical prediction of thermoplastic material properties by developing an expeditious method to parameterizing a simple yet surprisingly powerful coarse-grained bisphenol-A polycarbonate model which goes beyond previous coarse-grained models and successfully reproduces the thermal expansion behavior, the glass transition temperature as a function of the molecular weight, and several elastic properties.

CPP 20.31 Mon 17:30 Poster A

Structure-Property Relationships of Hyperbranched Polyamine ester/Ka-DCA nanocomposites. — •Shereen Omara[1,2], Mona H Abdel Rehim[2], Gamal Turky[2], Sherif Madkour[1], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und-prüfung (BAM), — [2]National Research Centre (NRC), 33 El Behouth St., Dokki, Giza, P.O.12622, (Egypt)

Hyperbranched polyamine ester (HPAE)/ kaolinite nanocomposites were papered via an ex situ (solution-based) method. The kaolinite has been modified by dodecylamine (DCA). SAXS measurements revealed that the Ka interlayer space increased from 0.71 to 3.6 nm-1. A partly exfoliated structure of the HPA/Ka-DCA nanocomposites was proved by SAXS and TEM. By a combination of BDS and SHS, the relaxation properties of the nanocomposites were investigated in dependence on frequency and temperature. The activation energies of γ-relaxation for the nanocomposites were lower than the values found for the pure HPAE. The segmental dynamics (α- relaxation) was found to be screened out by the conductivity contribution, while it was retrieved by SHS employing AC-chip calorimetry. The confinement effect of the Ka-DCA nanofillers reduces the glass transition temperature Tg and enhances, meanwhile, the electrical conductivity of the polymer. By comparing the temperature dependence of the dynamic glass transition measured with SHS and that of the dc conductivity measured by BDS, a decoupling in their temperature dependencies was found.

CPP 20.32 Mon 17:30 Poster A

Dynamic Properties of Multiblock Copolymers — •Fabian Berressem, Friederike Schmid, and Arash Nikoubashman — Institute of Physics, Johannes Gutenberg University Mainz

The ability of copolymers to self-assemble into well-defined nanostructures has been of enormous importance in academic studies as well as in industry. This remarkable property makes it possible to create large volumes of materials with specific nanostructures and tailored properties. Previous research has focused mainly on diblock copolymers, as these macromolecules are relatively easy to produce. However, recent advances in chemical synthesis have made it possible to create more complex polymers such as multiblock copolymers. Self-assembled structures of multiblock copolymers contain many loops and bridges, which can drastically alter the rheological properties of the polymer melts compared to simple diblock copolymer systems. The microscopic arrangement of the individual polymers, and thus the distribution of loops and bridges, strongly depends on the specific polymer properties as well as the employed manufacturing processes, e.g., solvent casting or spray coating. Therefore, it is crucial to consider the self-assembly of the chains on a microscopic level to fully understand the macroscopic flow properties of the melts. To this end, we combine self-consistent field theory and molecular dynamic simulations of Lennard-Jones chains. Our simulations reveal that the number of loops and bridges increases with the number of blocks in a copolymer. Further we study how the order of the self-assembled structures is improved by applying external fields, such as substrate patterning or shear.

CPP 20.33 Mon 17:30 Poster A

Evaluating thermal diffusion forced rayleigh scattering experiments with polydisperse polymers — •Bastian Pur and Werner Köhler — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany

The Soret effect (thermophoresis) describes a diffusion flux that is driven by a temperature gradient in a multicomponent mixture. By means of thermal diffusion forced rayleigh scattering (TDFRS), which is a holographic grating technique, one can obtain the collective (Fickian) diffusion coefficient D, the thermal diffusivity D_{th}, the Soret coefficient S_T and the thermal diffusion coeffcient, also known as the thermophoretic mobility, D_T. Measurements with binary mixtures, e.g. polymer solutions, can be evaluated with an working equation deduced from the linear response theory. This works well for monodispers polymers, but there are discrepancies due to polydispersity. Polydispersity was obtained by dynamic light scattering experiments, which yields the hydrodynamic radii distribution. From the initial rise of the concentration signal of TDFRS measurements, we can calculate the thermal diffusion coefficient D_T, even for polydisperse polymers.

CPP 20.34 Mon 17:30 Poster A

Quantum currents and pair correlation of electrons in a chain of localized dots — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP)Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The quantum transport of electrons in a wire of localized dots by hopping, interaction and dissipation is calculated and a representation by an equivalent RCL circuit is found. The exact solution for the electric-field induced currents allows to discuss the role of virtual currents to decay initial correlations and Bloch oscillations. The dynamical response function in random phase approximation (RPA) is calculated analytically with the help of which the static structure function and pair correlation function are determined. The pair correlation function contains a form factor from the Brillouin zone and a structure factor caused by the localized dots in the wire. Eur. Phys. J. B 90 (2017) 53

CPP 20.35 Mon 17:30 Poster A

Covalent dye functionalization of single-walled carbon nanotubes — •Gririraj Manoharan[1], Henrik Flötotto[2], Petra Bösel[1], René Wieczorek[1], Jan Kurzhals[1], Paul Kögerler[2], Wolfgang Harneit[1], Claire Besson[3], and Carola Meyer[1] — [1]Fachbereich Physik, Universität Osnabrück, Deutschland — [2]Institut für Anorganische Chemie, RWTH Aachen, Deutschland — [3]Department of Chemistry, The George Washington University, Washington, DC 20052, USA

Dye-functionalized carbon nanotubes (CNTs) have great potential for application in light-harvesting devices, in optical sensors, and in biosensing. Covalent attachment allows for high selectivity and stability of the reaction. It can be applied after a CNT has been contacted with electrodes to avoid surface or contact contamination. Our goal is to use CNTs as containers to place spin carriers next to shallow NV centers in diamond for quantum sensing.

We present covalent functionalization of single-walled CNTs with the Alexa Fluor® 594 dye, characterizing the individual steps of the chemical route. Dye-functionalized CNTs are dispersed on oxygen-terminated diamond and located by their fluorescence for co-localization with NV centers. An open question is whether a CNT in the vicinity of a shallow NV center quenches NV luminescence. We check this by monitoring the fluorescence of the stable color centers during bleaching of the dye molecules.

CPP 20.36 Mon 17:30 Poster A

Simulation of lithium-ion model batteries: A lattice Monte Carlo approach — •Alina Wettstein, Oliver Rubner, and Andreas Heuer — Institut für Physikalische Chemie, Münster

A great variety of theoretical approaches seeks to unravel the intrinsically multiscale and hence substantially complex behaviour of a battery cell. For the individual components such as electrolytes or electrodes atomistically resolved simulation techniques, e.g. molecular dynamics (MD) simulations, can be used. For the understanding of the whole cell continuum approaches have been developed. Here we present a lattice Monte Carlo (MC) model, which aims at simultaneous consideration of molecular-level properties and entire cell operation. Our MC model is designed as a modular system and includes the internal electrochemical processes as well as the particle motion given the relevant interactions and rates within a cell. We compute the experimentally accessible properties of a battery, such as voltage and capacity, for a minimum input of external parameters, i.e. diffusion coefficients that have been obtained from MD simulations. By means of this simplified, but yet highly flexible approach it is possible to further understand the basic principles of lithium-ion batteries.

CPP 20.37 Mon 17:30 Poster A

Incorporating chemical reactivity into classical molecular dynamics simulations — •Myra Biedermann[1], Diddo Diddens[2], and Andreas Heuer[1,2] — [1]Institute of Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster, Germany — [2]Helmholtz-Institut Münster (HI MS), Corrensstraße 46, 48149 Münster, Germany

We investigate the molecular transport and reaction processes at the interface between electrode and electrolyte in lithium ion batteries. More specifically, we are interested in the microscopic mechanisms which lead to the initial formation of the Solid Electrolyte Interphase (SEI) and the formation of dendrites in lithium ion batteries. For this purpose, we are working on incorporating chemical reactivity into classical molecular dynamics (MD) simulations by introducing reactive steps additionally to the MD steps. Our methodological approach is inspired by recent work of Takenaka et al. [1]. By doing so, we aim at developing a simulation method that incorporates chemical reactivity in a simple but realistic manner while retaining the time and length scales of standard MD simulations. The concepts are verified for a simple model system.

[1] N. Takenaka, Y. Suzuki, H. Sakai und M. Nagoaka, The Journal of Physical Chemistry C, pp. 10874-10882, 2014

CPP 20.38 Mon 17:30 Poster A

Finite-Size Effects in Molecular Dynamics Simulations of Ionic Liquids — •Diddo Diddens[1], Volker Lesch[1], Andreas Heuer[1,2], and Jens Smiatek[1] — [1]Helmholtz-Institut Münster, Ionics in Energy Storage (IEK-12), Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany — [2]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany

Ionic liquids (ILs) have recently gained significant interest due to their potential application as electrolytes for batteries and supercapacitors or as solvents for catalysis or CO_2 capture. Due to the fact that the properties of a given IL strongly depend on the detailed chemical interactions between cations and anions, molecular dynamics (MD) simulations are frequently employed to gain deeper insights on the microscopic level. However, with this technique, one typically is limited to rather small (albeit periodic) systems, which significantly affects the ion transport properties [1]. While analytical finite-size corrections exist for the self-diffusion coefficient [1-3], the impact of the system size on the conductivity is more intricate. In this contributribution, we utilize MD simulations in order to characterize the distance-dependent motional ion correlations contributing to the overall conductivity, and study how these correlations change with the system size. In addition, we rationalize our findings by analytical arguments.

[1] S. Gabl *et al.*, *J. Chem. Phys.*, **2012**, 137(9), 094501
[2] B. Dünweg, K. Kremer, *J. Chem. Phys.*, **1993**, 99(9), 6983
[3] I.-C. Yeh, G. Hummer, *J. Phys. Chem. B*, **2004**, 108(40), 15873

CPP 20.39 Mon 17:30 Poster A

Tuning and Suppressing the Conduction of Ionic Liquids by Confinement in Nanoporous Metal-Organic Frameworks — Anemar Bruno Kanj[1], Rupal Verma[1], •Modan Liu[2], Wolfgang Wenzel[2], and Lars Heinke[1] — [1]Karlsruhe Institute of Technology (KIT), Institute of Functional Interfaces (IFG) — [2]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology (INT)

Ionic liquids (IL) are room-temperature molten organic salts and metal-organic frameworks (MOFs) are nanoporous functional-material platforms compound of metal ions and organic linkers. The composite of both IL and MOF is intriguing and has huge potentials for nanoscale electronic devices as batteries or sensors.

IL embedded in MOFs is known to have properties deviating from bulk phase solution. Experiment shows molar conductivity of IL can see a drastic 3-orders-of-magnitude drop with respect to bulk phase conductivity when heavily loaded into the MOF, filling MOF pores.

Here, employing molecular dynamics (MD) simulations we investigate molar conductivity with various loading factors of [BMIM][NTf2] in HKUST-1. Result suggests dedicated and homogeneous flows of cation and anions are formed when bulk-phase solution is exposed external electric field, whereas, embedded in HKUST-1, cations and anions are forced to share channels inside MOF. Increasing loading of IL, mobility of ions becomes hindered as the aperture between MOF pores limits the flow. With higher loading, transient jamming and eventually a jammed layer of IL is formed, leading to the drastic drop in molar conductivity. Statistics of MD confirm measurements from experiment.

CPP 20.40 Mon 17:30 Poster A

Multi-Phase Transition Behavior of Highly Conductive Polybromide Ionic Liquids — •Falk Frenzel[1], Karsten Sonnenberg[2], Sebastian Hasenstab-Riedel[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Leipzig, Germany — [2]Freie Universität Berlin, Berlin, Germany

Over the last three decades Ionic Liquids (ILs) have reached such a remarkable scientific interest that nowadays this class of materials comprise a million dollar market being commercially used in application areas like medicine, energy technology and synthetic chemistry. Even though most scientific questions for 'standard' ILs have been addressed and already answered the novel subclass of (poly) halogenide Ionic Liquids opens the window to unique properties like multiple phase transitions. In order to study them as well as the molecular dynamics and charge transport mechanism X-ray scattering, broadband dielectric spectroscopy (BDS) and differential scanning calorimetry (DSC) have been employed to six different samples consisting of asymmetrical ammonium cations in composition with tribromide respectively nonabromide anions. The current study unravels three molecular relaxation processes, whereat one is assigned to the dynamic glass transition (DGT) while the other both are secondary relaxations, as well as the primarily charge transport mechanism that is determined to be a DGT assisted hopping process. Furthermore, the at room temperature remarkably high DC-conductivity (>10 mS/cm) is strongly dependent on the thermally history below 300K due to distinct hystereses of the phase transitions.

CPP 20.41 Mon 17:30 Poster A

Inter- and Intramolecular Interactions in an Extraordinary Conductive Polymeric Ionic Liquid — •Arthur Markus Anton, Falk Frenzel, and Friedrich Kremer — Peter Debye Institute for Soft Matter Physics, Leipzig University

Polymeric ionic liquids (PILs) combine the advantages of neat ionic liquids, such as electrochemical and thermal stability or high ion conductivity, with the benefits of polymers like well-controllable processing and structure formation conditions. Due to these advantages, PILs are of principal importance for applications like super-capacitors or battery media. Recently, it has been reported from a novel PIL which exhibits the highest dc-conductivity at temperatures below 100°C and –contrary to the common dogma– an intensified charge transport with *rising degree of polymerization* [1]. In order to shed light on the origin of the material's extraordinary performance, we examined temperature-dependent FTIR spectroscopy in combination with broadband dielectric spectroscopy. On the one hand the pure cation exhibits a lower dc-conductivity ($2 \cdot 10^{-9}$ vs. $2 \cdot 10^{-7}$ S/cm at $T_g + 50$ K) than the polymeric system, on the other hand an extensive H-bond network is established, which is characterized through a distinct hysteresis in cooling-heating cycles demonstrating the stabilization of the structure through intermolecular interactions. Thus, the interplay between polymer and cations leads to the enhanced dc-conductivity which is higher than that of a separated part of the system. [1] F. Frenzel, A. M. Anton, F. Kremer et al., Macromolecules 50 (2017) 4022-4029

CPP 20.42 Mon 17:30 Poster A

1H and 19F PFG NMR of choline-based ionic liquids in bulk and in carbon fibers — •Emmanouil Veroutis, Steffen Merz, Markus Gehring, Rüdiger Eichel, and Josef Granwehr — Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research - Fundamental Electrochemistry (IEK-9), 52428 Jülich, Germany

In recent years great interest has been attracted by room temperature ionic liquids (RTILs) due to their potential as new media for organic, catalytic and electrochemical applications. Given their interesting properties, such as very low vapor pressure, non-flammability, high thermal stability and wide electrochemical window, ILs are proposed as electrolytes for batteries. Despite of this research attention, electrolyte ILs and their interactions with electrodes in battery systems still remain poorly characterized.

In this study we present 1H and 19F Pulsed Field Gradient (PFG) NMR measurements on choline-based ionic liquids in bulk as well as confined in electrospun carbon fibers. The self-diffusion coefficients of the cation and the anion have been measured and correlated with electrochemical parameters, such as molar conductivity, transference numbers and ionicity. Furthermore, the interactions of cation and anion, but also the interaction with the carbon fibers have been examined by means of Nuclear Overhauser Effect Spectroscopy (NOESY) NMR, which provides through-space correlations between nearby nuclei. Finally, the influence of water on the physicochemical parameters of the studied ionic liquids has also been addressed by NMR.

CPP 20.43 Mon 17:30 Poster A

Static and Dynamic Properties of [C_2Mim][NTf_2] Ionic Liquid on Neutral Sapphire Surface — •Nataša Vučemilović - Alagić[1,2], Daniel Berger[4], Jens Harting[4,5], Christian Wick[1,3], David M. Smith[1,2], and Ana-Sunčana Smith[1,2,3] — [1]EAM, Cluster of Excellence, FAU, Erlangen, Germany — [2]Ruđer Bošković Institute, Zagreb, Croatia — [3]Institute for Theoretical Physics I, FAU, Erlangen, Germany — [4]Forschungszentrum Jülich GmbH, Helmholtz-Institut Erlangen-Nürnberg for Renewable Energy — [5]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

In the last decades it has become a common practice to use ionic liquids films in the context of catalysis. A particular advantage of these systems is their low vapour pressure and powerful solvation . Understanding the solvent effects both in the context of interface wetting and chemical reactions is vitally important for the technological applications of ILs, however, the understanding of these processes is still not satisfactory. To address this problem, we employ atomistic molecular dynamics (MD) simulations and investigate the behaviour of the archetypical imidazolium-based IL [C_2Mim][NTf_2]. We systematically study the role of the IL model introduced through the force field, and determine their static and dynamic properties at interfaces with a hydroxylated sapphire or vacuum. We use this model to study the structuring of IL and the changes of its transport properties as a function of the distance from the interface of choice.

CPP 20.44 Mon 17:30 Poster A

Strong Polyelectrolytes and Specific Counterion Condensation Effects: A Molecular Dynamics Simulation Study — •anand narayanan krishnamoorthy[1], christian holm[1], and jens smiatek[2] — [1]Institute for Computational Physics - University of Stuttgart — [2]Institute of Energy and Climate Research (IEK) - Forschungszentrum Jülich

We study specific counterion condensation effects in aqueous solution for monovalent alkali and halide ions with model polyelectrolyte using atomistic Molecular Dynamics simulations. Our results reveal significant differences between the individual ion types distributions around a rigid artificial strong polyelectrolyte. The results of the simulations demonstrate that mean-field theories which disregard the molecular nature of the solvent are inappropriate to explain the observed deviations. Furthermore we studied specific counterion condensation effects in non aqueous solvents like DMAc and methanol which provides an insight into specific ion effects in non aqueous medium and helps in understanding hoffmeister effects in non aqueous systems. Our results validate the strong dependence of condensation properties on ion chemical details and solvent effects in addition to electrostatic interactions.

CPP 20.45 Mon 17:30 Poster A

Roughness and Salt Annealing in a Polyelectrolyte Multilayer — •Amir Azinfar[1], Sven Neuber[1], Jiri Vanecek[2], Maria Vancova[2], Viteslav Stranak[2], and Christiane A. Helm[1] —

[1]Inst. f. Physics, Greifswald University, Germany — [2]Fac. of Science, University of South Bohemia, Ceske Budejovice, Czech Republic

The surface roughness of polyelectrolyte multilayers made from poly(diallyldimethylammonium chloride) (PDADMA) and poly(styrene sulfonate) (PSS,10.6 kDa) increases with the number of deposition steps until the linear growth regime is reached; then it is constant. AFM and Electron microscopy show the formation of micrometer-sizes features. The wavelength of the roughness features is approximately proportional to film thickness, which supports a mechanism whereby roughness is generated by anisotropic shrinking due to dehydration. Due to the viscous response of polyelectrolyte complexes the surface features are possibly better described as *damped* creases, where a small amount of flow is allowed in the most stressed regions. Annealing in high salt decreases in the long term the roughness.

CPP 20.46 Mon 17:30 Poster A

Electrostatic bending response of a helical chain of charges — •Alexandra Zampetaki[1], Jan Stockhofe[1], and Peter Schmelcher[1,2] — [1]Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

We explore the electrostatic contribution to the bending response of a chain of identical charged particles confined on a finite helical filament. We analyse how the energy difference ΔE between the bent and the unbent helical chain scales with the length of the helical segment and the radius of curvature and identify features that are not captured by the standard notion of the bending rigidity, normally used as a measure of bending tendency in the linear response regime. Using instead ΔE to characterize the bending response of the helical chain for low values of the radius-to-pitch ratio we find that it exhibits interesting oscillations with the number of particles, encountered for commensurate fillings. These oscillations yield length-dependent oscillations in the preferred bending direction of the helical chain of charges. We show that the origin of such oscillations is the non-uniformity of the charge distribution caused by the long-range character of the Coulomb interactions and the finite length of the chain.

CPP 20.47 Mon 17:30 Poster A

Interactions among Spherical Polyelectrolyte Brushes in Concentrated Aqueous Solutions — •Yunwei Wang[1,2], Regine von Klitzing[1], and Xuhong Guo[2] — [1]Technische Universität Darmstadt,Darmstadt,Germany — [2]East China University of Science and Technology,Shanghai,China

Interactions among annealed spherical polyelectrolyte brushes (SPB) in concentrated aqueous dispersion are studied by rheology measurements, small angle X-ray scattering (SAXS) and wide X-ray scattering (WAXS). The SPBs consist of a solid poly(styrene) core and a shell of poly(acrylic acid) (PAA). The effect of SPB concentration; pH; salt concentration have been explored. At 12 wt-%, SAXS spectra show a new peak which is assumed to be caused by overlapping polyelectrolyte chains. They are associated and form locally ordered structures which reflects the enhanced interactions among SPB. The locally ordered structures of brushes are proved by WAXS. For further validation of the interaction between the PAA chains and its influence on the emulsion rheological properties, the concentration of 12wt% brushes of the different pH and salt concentration were studied.

CPP 20.48 Mon 17:30 Poster A

Silica Coating for Stabilization of Tubular J-aggregates — •Katherine Herman, Stefan Kirstein, and Jürgen P. Rabe — Humboldt Universität zu Berlin Institut für Physik, Berlin, Germany

Cyanine dyes are remarkable for their ability to form supramolecular aggregates with both diverse morphologies as well as the signature narrow absorbance and emission bands of J- or H- aggregates. Cyanine dyes that form one dimensional nanostructures are of particular interest not only for their potential as light harvesting and energy transport structures, but also as systems for fundamental linear and non-linear spectroscopic studies. However, several powerful methods for investigating optical and energy transfer properties require that the sample be stable under dry and low pressure conditions. A possible means of stabilization is inorganic coating of the water soluble aggregates. Here we present an approach for a silica coating to stabilize tubular aggregate of amphiphilic cyanine dyes for dry and low pressure investigations. An initial monolayer of silica is formed by ionic self assembly of a functionalized organosilane on the aggregate surface. Further shell growth is achieved by gradual addition of a second organosilane under basic conditions. Evidence for silica shell growth on the aggregate comes from fluorescence spectroscopy and atomic force microscopy.

CPP 20.49 Mon 17:30 Poster A

Growth Kinetics and Molecular Mobility of Irreversibly Adsorbed Layers in Thin Polymer Films — •Marcel Gawek and Andreas Schönhals — Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin

In well-annealed thin polymer films, with non-repulsive polymer/substrate interactions, an irreversibly adsorbed layer is expected to form. These adsorbed layers have shown great potential for technological applications. However, due to the hard accessibility of these buried layers in thin films, their growth kinetics and molecular dynamics are still not fully understood. Here, the irreversibly adsorbed layers of homopolymer thin films are revealed by solvent-leaching experiments. First, the growth kinetics of these layers is investigated as a function of original film thickness and annealing times. The thickness, topography and quality of the adsorbed layer is determined with Atomic Force Microscopy (AFM). Secondly, the molecular mobility of the adsorbed layer is investigated with Broadband Dielectric Spectroscopy (BDS) with high-resolution analyzers. A recently developed nanostructured capacitor (NSC) is employed to measure the adsorbed layers with a free surface layer. The results are quantitatively compared and discussed with respect to recently published work.

CPP 20.50 Mon 17:30 Poster A

Phase Separation in Phthalocyanine-Fullerene Co-Deposited Thin Films — •Berthold Reisz, Giuliano Duva, Valentina Belova, Clemens Zeiser, Santanu Maiti, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — Universität, Tübingen, Deutschland

Co-deposited blends of copper phthalocyanine (CuPc) and Buckminster fullerenes (C60) are well known phase separating donor-acceptor systems exhibiting (compared to successive deposition) a dramatic modification of the thin film architecture with improved solar cell performance [1,2]. Till today, neither the assignment of morphological features to distinct molecular phases nor the separation processes are known. We followed the growth of pure and blended thin films by in situ real-time X-ray reflectivity and found material dependent roughening during the growth. Post growth X-ray diffraction at two grazing angles of incidence revealed an accumulation of C60-molecules at the surface, which may correspond to the tall features seen from atomic force microscopy. Further experiments aiming at a deeper insight into the phase separation processes are planned.

[1] P. Sullivan et al., Appl. Phys. Lett. **84** (2004)
[2] S. Heutz et al., Sol. Energ. Mat. Sol. Cells **83** (2004)

CPP 20.51 Mon 17:30 Poster A

Thin films of ultrahigh molecular weight diblock copolymers — •Wei Cao[1], Senlin Xia[1], Michael Appold[2], Markus Gallei[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]TU Darmstadt, Ernst-Berl-Institute for Technical and Macromolecular Chemistry, 64287 Darmstadt

Block copolymer self-assembly has attracted considerable attention for many decades because it can yield ordered structures in a wide range of morphologies, including spheres, cylinders, bicontinuous structures, lamellae, vesicles, and many other complex or hierarchical assemblies. So far, most studies have used block copolymers with low or medium scale molecular weight. Due to scaling of the micro-phase separation structure with the molecular weight of the the block copolymers, large periods (about 100 nm) can be achieved with ultrahigh molecular weight (UHMW) block copolymers (Mn > 800 kg/mol). In thin film geometry this implies a confinement of the polymers. For polystyrene-block-polymethylmethacrylate UHMW diblock copolymers we prepare thin films. Different thermal and solvent post-treatments are studied to achieve highly ordered micro-phase separation structures. The film morphology is probed with atomic force microscopy (AFM), scanning electron microscopy (SEM) and grazing incence small angle x-ray scattering (GISAXS).

CPP 20.52 Mon 17:30 Poster A

Printed low bandgap polymer films — •Xinyu Jiang and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Printing of low bandgap polymer films is of interest in organic photovoltaics. Roll-to-roll processing and large-area processability on low cost together with flexible substrates make conjugated polymer-based organic solar cells extremely attractive as a cost-effective solution to today's energy-shortage problem. We study printed mixtures of the low-bandgap polymer PTB7 with the fullerene derivate PCBM with respect to optical absorption and electrical properties. The film structure and morphology is proved with atomic force microscopy (AFM), scanning electron microscopy (SEM) and grazing incidence small angle x-ray scattering (GISAXS).

CPP 20.53 Mon 17:30 Poster A

Investigation of the impact of antifoam agents on lipid membranes by XRR and BAM — •Mike Moron, Susanne Dogan, Julia Nase, Michael Paulus, and Metin Tolan — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany

The control of foam by means of antifoam agents is of great importance in a number of applications. For example, the oral administration of simethicone is prescribed in the case of surfactant intoxication and also in order to prepare patients for coloscopy. In both cases, simethicone reduces the amount of foam. Other domains where antifoam agents play a role are for example the kraft pulp process, radioactive waste treatment, and machine detergents. While the macroscopic behaviour of liquid systems containing antifoam agents and lipids is well understood, the modes of action on the molecular scale are not. Various theories were established to describe the molecular mechanisms, but the actual behaviour showed up to be strongly dependent on the system under investigation. We present a surface pressure-dependent in-situ X-ray reflectometry and Brewster-angle microscopy study on Langmuir-Blodgett monolayers consisting of different lipids and simethicone. Both the X-ray reflectivities and the BAM-measurements were performed at the liquid-air interface. The reflectivities provide information on the vertical structure of the systems, whereas the BAM-measurements reveal the lateral structure. With this combined information, it is possible to analyse the different models.

CPP 20.54 Mon 17:30 Poster A

Morphologies in liquid-liquid dewetting — •Roghayeh Shiri[1], Ralf Seemann[1], Dirk Peschka[2], and Barbara Wagner[2] — [1]Experimental physics, Saarland University, Saarbrucken, Germany — [2]Weierstrass Institute, Mohrenstr 39, Berlin, Germany

We study the dewetting of thin nanometric thin polystyrene (PS) films from liquid polymethyl-methacrylate (PMMA) substrates. In order to induce dewetting the PS/PMMA samples are heated above the glass transition temperature of both polymers. After a few minutes circular holes appear in the PS film and their radii grow with time and finally coalescence leading to a set of droplets on the substrate.

The considered mechanism leading to the symmetry breaking of the initially flat film is called spinodal dewetting, which is initiated due to the growth of thermally activated surface waves. The spinodal rupture of the liquid film results in a dewetting pattern of *hills and gullies* with a certain preferred wavelength λ in both liquid/air and liquid/liquid interfaces leading eventually to the formation of holes after a certain time t. Interestingly, the deformation of the liquid/liquid interface is larger than that of the liquid/air interface due to the lower surface tension. According to theoretical predictions, can the deflection of both interfaces be in phase or antiphase which determines the dewetting pathway.

In this study we experimentally measured the preferred wavelength λ and holes distance and we monitor deformation of interfaces by atomic Force Microscopy. Ultimately, the result of experimental observations will be compared with theoretical modelling.

CPP 20.55 Mon 17:30 Poster A

Structure formation of organic molecules on dielectric surfaces — •William Janke and Thomas Speck — Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany

When buckminsterfullerenes (C_{60}) are deposited upon a substrate by means of molecular beam epitaxy, many different structures can form depending on the substrate in use and the experimental conditions. Calcium fluoride (CaF_2) as a substrate is particularly interesting since its interaction with C_{60} is slightly weaker than the C_{60}-C_{60} interaction, which leads to very interesting types of two-layered clusters. These clusters and other properties of the C_{60}-CaF_2 system have been observed in experiments [1]. To further the understanding of such deposition and diffusion systems, we study the diffusion and self-assembly of C_{60} on CaF_2(111) by means of MD and KMC simulations as well as theoretical considerations to build a comprehensive model for this system.

[1] Felix Loske, Jannis Lübbe, Jens Schütte, Michael Reichling, and Angelika Kühnle. Quantitative description of C_{60} diffusion on an insulating surface. Phys. Rev. B, 82:155428, Oct 2010.

CPP 20.56 Mon 17:30 Poster A

Model-Free Thickness Determination of Nanoscale Foam Films using FTIR spectroscopy — •Eric Weissenborn and Björn Braunschweig — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany

The thin-film-pressure balance (TFPB) technique allows to determine intermolecular forces in free standing foam films. In order to calculate the surface potential of charged air/water/air interfaces, DLVO theory is applied where the correct size of the water core is extremely important. However, in the classical approach where the thickness is determined interferometrically, models of the adsorbate layer and its thickness have to be applied. In order to address the thickness of foam films, we have extended the abilities of a classical TFPB by combining interferometric UV/Vis spectroscopy and transmission IR spectroscopy in a single setup. Particularly, the coupling of a TFPB to a FTIR spectrometer allows to record IR spectra of foam films. From IR transmission spectra, we can not only accurately determine the foam film thickness as function of disjoining pressure by looking at the water O-H absorption bands, but can also determine their composition with the help of IR vibrational bands and their attribution to specific molecular vibrations. In order to demonstrate the proof of concept, we present disjoining pressure isotherms of cetyltrimethylammonium bromide (C_{16}TAB) foam films at 0.9 and 0.1 mM concentrations and compare the film thicknesses from both interferometric UV/Vis and infrared spectroscopy.

CPP 20.57 Mon 17:30 Poster A

Real-time XRR study of protein adsorption at the solid-liquid interface guided by multivalent ions — •Simon Schönberg[1], Madeleine Fries[1], Alexander Hinderhofer[1], Fajun Zhang[1], Robert M. J. Jacobs[2], Maximilian W. A. Skoda[3], and Frank Schreiber[1] — [1]Institute for Applied Physics, University of Tübingen, 72076 Tübingen, Germany — [2]Department for Chemistry, Chemistry Research Laboratory, University of Oxford, OX1 3TA, United Kingdom — [3]Rutherford-Appleton Laboratory, ISIS Facility, Didcot

The unique influence of multivalent ions on the phase behaviour of protein solutions has been subject of past and current research [1]. Moreover, the influence of multivalent ions (Y^{3+}) on the adsorption behaviour of protein (BSA) at the solid-liquid interface and thus the connection of bulk and interface behaviour was recently established [2]. In this context, we designed a new liquid cell for measurements at the solid-liquid interface *via* X-ray reflectivity (XRR). This setup allows real-time measurements of protein adsorption through the use of a molybdenum source. We successfully established this new XRR setup, which enables us to reproduce previous outcomes of ellipsometry measurements on multivalent ion-tuned protein adsorption. Further it allows to study more parameters such as temperature dependency of our system, surface roughness and surface coverage/density and thus promotes a more detailed understanding of protein adsorption tuned by multivalent ions.

[1] Zhang, F. et al., Pure Appl. Chem (2014), 86, 191-202.
[2] Fries, M. R. et al., Phys. Rev. Lett. (2017), in print.

CPP 20.58 Mon 17:30 Poster A

Dynamics of nanoscopically confined PVME in thin films of an asymmetric PVME/PS blend — •Paulina Szymoniak, Sherif Madkour, and Andreas Schönhals — BAM Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin (Germany)

In recent years, substantial efforts have been devoted to investigating nanoscopic confinement of polymers, and its effect on glassy dynamics. Broadband Dielectric Spectroscopy (BDS) was used to study the dynamics of ultra-thin films of PVME/PS 50/50 wt% blend, employing a novel nano-structured capacitor sample arrangement. The investigated system shows a complex dynamic behavior. First, an α-relaxation, related to a bulk-like layer was found. Second, an α'-relaxation was observed, characteristic for dynamically asymmetric blends, where the out of equilibrium dynamics is attributed to weakly-cooperative PVME segments relaxing within a frozen environment of PS segments. Thirdly, for thinnest films, an Arrhenius-like process was dominant in the dielectric spectra, indicating localized fluctuations of the segments. Relaxation rates of this process resembled that of the degenerated α-relaxation of the adsorbed layer, found for pure PVME [1], thus it was assigned accordingly. For thinnest films, this process undergoes a further confinement, due to the topological constraints, introduced by PS. Such multiple confinement effect has not been reported for ultra-thin films of polymer blends, before this study [2]. [1] Madkour, S. et al. ACS Appl. Mater. Interfaces 2017, 9, 7535. [2] Madkour, S. et al. ACS Appl. Mater. Interfaces 2017, 9, 37289

CPP 20.59 Mon 17:30 Poster A

Competition of mobilization and immobilization effects of segmental dynamics in epoxy/Boehmite nanocomposites — •Paulina Szymoniak, Dorothee Silbernagl, Media Ghasem Zadeh Khorasani, Heinz Sturm, and Andreas Schönhals — BAM Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin (Germany)

The interphase between the inorganic filler and the polymer matrix is considered as one of the most important characteristics of inorganic/polymer nanocomposites. The segmental dynamics of this interphase is expected to be altered as compared to the pure matrix, which might percolate into the entire system. For instance, it was found that a so-called Rigid Amorphous Phase (RAF) is formed by adsorption of segments onto the nanoparticles, yielding in their immobilization. The RAF is available from the decrease of the specific heat capacity step ΔCp in the glass transition region of the nanocomposites. Here, precise Temperature Modulated DSC (TMDSC) was employed to study ΔCp of epoxy/Boehmite nanocomposites with different nanofiller concentrations. Surprisingly, the investigated system showed an increase of ΔCp with increasing filler concentration up to 10 wt%. This implies an increased fraction of mobile segments, and is in accordance with the found decreased value of the glass transition temperature Tg. Although for higher filler contents Tg further slightly decreases, ΔCp decreases in contrary, indicating a formation of RAF. This behavior was discussed as a competition of mobilization effects, due to an incomplete crosslinking reaction, and the formation of RAF.

CPP 20.60 Mon 17:30 Poster A

Temperature Dependent Photoluminescence Studies on Zinc Phthalocyanine Thin Films — •Gabriel Freiherr von Eyb[1], Maximilian Frank[1], Simon Wiegand[1], Sebastian Hammer[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

In recent years, there has been many opto-electronic applications implementing zinc phthalocyanine (ZnPc) as active organic component [1]. For the performance of those devices the temperature dependent optical behaviour of ZnPc is of relevance but has not been investigated to a sufficient extent.

In this work we analyse the spectral photoluminescence (PL) of ZnPc thin films in a temperature range of 20 to 360 K. The films under study were prepared by vacuum sublimation on glass and SiO2 substrates. Optical excitation of excitons in the ZnPcs Q-band reveals two main emission components whose intensity varies with temperature. The high energy component experiences a decrease in intensity towards lower temperatures, almost vanishing completely at 20K. The low energy emission decreases as well, but not at the same extent. Combining the temperature dependent PL data with (room temperature) life-time measurements, we will address the role of singlets and triplets in the radiative and non-radiative relaxation processes in ZnPc and discuss possible similarities with a thermally activated delayed fluorescence mechanism.

[1] M. Brendel, et al., Adv. Func. Mater. 25 (2015) 1565

CPP 20.61 Mon 17:30 Poster A

Quantifying surface potentials at liquid-gas interfaces from vibrational SFG spectroscopy — Eric Weissenborn, Felix Schulze-Zachau, Georgi Gochev, •Natalia García Rey, and Björn Braunschweig — Institute of Physical Chemistry, Westfälische Wilhelms-Universität Münster, Corrensstrasse 28/30, 48149 Münster, Germany

Knowing the double layer potential (ψ_0) of the liquid-gas surface is essential to analyze the mechanisms of foam stabilization. However, no straightforward method is available to measure ψ_0. The intrinsic negative charging of pure water surface is significantly modified by adsorbing ionic surfactants while non-ionic surfactants change only slightly the ψ_0-magnitude. Adsorption of cationic surfactants will first neutralize the surface negative charge and further will cause charge reversal. By mixing non-ionic and cationic surfactants, we can tune the negative/zero/positive ψ_0 at the air-water surface. On charged interfaces, the SFG intensity depends not only on the 2^{nd}-order of susceptibility ($\chi^{(2)}$) but also on the 3^{rd}-order ($\chi^{(3)}$) due to impact of ψ_0. SFG spectroscopy used to quantifying the ψ_0 requires first its calibration to untangle the $\chi^{(2)}$ and $\chi^{(3)}$ from the spectra. ψ_0 is estimated from theoretical (DLVO) analysis of the disjoining pressure isotherm for a foam film as measured with the thin-film pressure balance (TFPB) technique. These experiments will allow for validation of data form OH-SFG spectra taken for isolated surface that can be applied to extract ψ_0-values. This is the first study to our knowledge that combines TFPB and SFG experiments for studying soft interfaces.

CPP 20.62 Mon 17:30 Poster A

Structure of ice/clay nanocomposites — •Hailong Li[1], Rika Unkelbach[1,2], Julian Mars[1,2], Ann-Christin Dippel[3], Olof Gutowski[3], Veijo Honkimäki[4], and Markus Mezger[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz — [2]Max-Planck-Institut für Polymerforschung, Mainz — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg — [4]ESRF-The European Synchrotron, Grenoble

Material properties of permafrost strongly depend on the texture of the confined crystalline ice and the properties the quasi-liquid premelting layer (qll) formed at ice/solid interfaces. The layered sheet silicates vermiculite and kaolin with high interface to volume ratios are ideal model systems to study interfacial melting in geologically relevant ice/clay composites. The crystalline ice fraction and its preferred orientation was determined by temperature dependent x-ray diffraction experiments. Well below the melting point of bulk water, the formation of a qll is observed. The temperature dependent thickness of this qll follows a logarithmic growth law. However, different coefficients are observed for the charged vermiculite and uncharged kaolin clays.

CPP 21: Focus: Smart Hydrogels and Hydrogel Based Devices I - organized by Gerald Gerlach, Walter Richtering and Thomas Hellweg

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

Topical Talk CPP 21.1 Tue 9:30 C 130

Superresolution microscopy of pNIPAM microgels — •Frank Scheffold[1], Gaurasundar Marc Conley[1], Philippe Aebischer[2], Sofi Nöjd[2], Marco Braibanti[1], and Peter Schurtenberger[2] — [1]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland — [2]Physical Chemistry, Department of Chemistry, Lund University, 221 00 Lund, Sweden

Microgels are among the most studied colloidal and polymeric systems of the past two decades. Swelling thermosensitive, poly(N-isopropylacrylamide) microgels by lowering the temperature provides a unique mechanism for controlling the porosity and size of colloidal particles on the nanoscale. As a consequence, these smart microgel particles are being considered for applications ranging from viscosity modifiers and sensing to drug delivery and as models for the glass and the jamming transition. Here, we present results from in-situ two-color superresolution microscopy of dye-labelled submicron sized pNiPAM microgels. We first demonstrate direct STochastic Optical Reconstruction Microscopy (dSTORM) to image single microgels in two and three dimensions, at different stages of the volume phase transition, with a lateral resolution of 30nm. We find that the swelling behaviour observed in real space matches quantitatively with results from traditional light scattering measurements in reciprocal space. Next, we study dye labelled tracer microgels embedded in dense microgel suspensions. As we increase the packing density we map out the different contributions that allow the dense packing of the soft microgels, due to deformation, interpenetration and compression.

CPP 21.2 Tue 10:00 C 130

Soft photonic crystals from core-shell mircogels — Astrid Rauh[1] and •Matthias Karg[2] — [1]Physical Chemistry I, University of Bayreuth, Universitaetsstr. 30, 95447 Bayreuth — [2]Physical Chemistry I, Heinrich-Heine-University Duesseldorf, Universitaetsstr. 1, 40204 Duesseldorf

Photonic crystals are well known for their fascinating angle-dependent opalescence. In contrast to hard sphere building blocks, crystals from soft spheres such as microgels allow for external actuation, e.g. melting and recrystallization induced by pH or temperature changes. In addition, soft spheres can be deformed and thus packing fractions well above the hard sphere limit are accessible. A drawback with respect to the optical diffraction of soft photonic crystals is the typically low refractive index modulation inside the material. This asks for pathways to increase the refractive index contrast in the periodic superstructure.

We prepared cm-sized soft photonic crystals from core-shell microgels with absorbing nanocrystal cores (Au nanoparticles) and systematically studied the crystal structure and diffractive properties. As non-absorbing references, we prepared pitted particles from the same microgel batches by dissolution of the nanocrystal cores. The resulting purely organic microgels allowed for a direct comparison of structural and optical properties. We identify the role of small absorbing nanocrystal cores and show options to alter the photonic behavior of soft photonic crystals in future studies.

[1] A. Rauh et al., Langmuir 2017, DOI: 10.1021/acs.langmuir.7b01595

CPP 21.3 Tue 10:15 C 130

Rational design of Ag@PS-PNIPAM core-shell nanoreactors with tunable activity for catalysis — •Daniel Besold[1], Sebastian Risse[1], Rafael Roa[1], Yan Lu[1,2], Joachim Dzubiella[1,3], and Matthias Ballauff[1,3] — [1]Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Germany — [2]Institut für Chemie, Universität Potsdam, Potsdam, Germany — [3]Institut für Physik, Humboldt-Universität zu Berlin, Germany

Nanoreactors containing metal nanoparticles embedded in stimuli-responsive polymers have recently emerged as promising catalytic systems. The polymer coating not only prevents nanoparticle aggregation but also controls the catalytic activity by changing the local environment for the reactants. For this work we synthetized thermosensitive core-shell nanoreactors, composed of a polystyrene core in a PNIPAM microgel shell, in which silver nanoparticles are immobilized. In this system, we study the catalytic reduction of 4-nitrophenol by borohydride ions. Our kinetic analysis is based on UV-Vis spectroscopic techniques. The spectra are deconvoluted by the Levenberg-Marquardt algorithm which provides us with the concentration-time dependency of the species involved in the reaction. We tune the catalytic activity of the silver nanoparticles by tuning the temperature of the system. We find two distinct regimes in the catalytic rate at temperatures below and above the volume transition of the PNIPAM shell. By means of a modified Langmuir-Hinshelwood mechanism which accounts for electrostatic effects on the reactant adsorption, we attribute the changes in the rate to changes in the reactant partitioning in the shell.

CPP 21.4 Tue 10:30 C 130

Smart core-shell microgel/silver nanoparticle hybrids as switchable catalysts — •Timo Brändel, Yvonne Hertle, and Thomas Hellweg — Physical and Biophysical Chemistry, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld

Hybrid materials combining the interesting properties of nanoparticles with stimuli responsive microgels have obtained considerable attention during the last decade. Our contribution focuses on core-shell microgels based on the monomers, *N*-isopropylacrylamide (NIPAM) *N*-isopropylmethacrylamide (NIPMAM) as core materials and *N*-*n*-propylacrylamide (NNPAM) as shell material. These microgels exhibit a very interesting linear phase transition region between the two volume phase transition temperatures (VPTTs) of the respective homopolymer microgels.

The particle architecture of the core-shell microgels is modified by copolymerization with acrylic acid (AAc) and by a variation of the cross-linker density of the core. These modifications in the core region of the core-shell microgels are important steps to tailor the microgel properties towards an excellent ability to stabilize nanoparticles.

Silver nanoparticles are generated *in situ* inside the core-shell microgel templates and their temperature dependent catalytic activity is studied by following the degradation of *p*-nitrophenole. The results display, that the use of the core-shell microgels is a versatile approach towards catalytic particles with a switchable catalytic activity.

CPP 21.5 Tue 10:45 C 130

Doping thermosensitive PNIPAM microgels with magnetic nanoparticles — •Marcus. U. Witt[1], Stephan Hinrichs[2], Melissa Hermes[3], Birgit Fischer[2], Annette Schmidt[3], and Regine v. Klitzing[1] — [1]Technische Universität Darmstadt, Institut für Festkörperphysik, Alarich-Weiss-Straße 10, 64287 Darmstadt — [2]Universität Hamburg, Institut für Physikalische Chemie, Grindelallee 117, 20146 Hamburg — [3]Universität zu Köln, Institut für Physikalische Chemie, Luxemburger Straße 116, 50939 Köln

Poly-N-isopropyl acrylamide (PNIPAM) based microgels are of high interest as model systems for thermo-responsive gel structures that exhibit a volume phase tran-sition temperature. First results with the loading of the microgels with magnetic nanoparticles (MNP) showed a small re-sponse of the particle volume to an external magnetic field under geometrical confine-ment [1]. Theoretical calculations predict a much bigger response. To investigate now the origin of this difference in response the MNP distribution inside the microgel is of interest.

Therefore gels of different internal polymer structure are synthesized: heterogeneously cross linked microgels (batch) and homo-geneously cross linked microgels (feeding) [2]. The MNP distribution is different in the two cases and is of interest for further investigations of the magnetic response for magnetic microgels particles.

References

[1] S. Backes, M. U. Witt, R. v. Klitzing, J. Phys. Chem. B 2015, 119, 12129-12137 [2] R. Acciaro, Langmuir, 2011, 27, 7917-7925

15 min. break

CPP 21.6 Tue 11:15 C 130

Film-coupled plasmonic arrays based on core-shell microgel particles — •Yannic Brasse[1], Mareen B. Müller[2], Matthias Karg[3], Christian Kuttner[1,4], Tobias A. F. König[1,4], and Andreas Fery[1,4] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Institute of Physical Chemistry and Polymer Physics, Hohe Str. 6, 01069 Dresden, Germany — [2]Physical Chemistry II, University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [3]Department of Physical Chemistry 1, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany — [4]Cluster of Excellence Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, 01062 Dresden, Germany

We study the optical properties of a metal-film-coupled gold nanoparticle system, separated by a Poly(N-isopropylacrylamide) (PNIPAM) layer, as cost-efficient and scalable platform for screening of plasmonic properties. As shown in earlier work, a monolayer of gold-core/PNIPAM-shell particles featuring a gradient in core-sizes, results in lateral variation of plasmonic resonances.[1] Coverage with a 35 nm gold layer induces plasmonic coupling between cores and the film. We study the tunability of the array by swelling of PNIPAM for various particle sizes, which reveals a reversible plasmonic shift of up to 40 nm. With this lithography-free method we produce a platform for systematic screening of fundamental optical effects and for application in surface plasmon resonance (SPR) sensing.[2]

[1] M.B. Müller et al., ACS Nano, 2014, 8, 9410 [2] Funding from ERC Starting Grant METAMECH-306686 is acknowledged

CPP 21.7 Tue 11:30 C 130

Water swelling and exchange kinetics of multi-stimuli responsive polymer thin films — •Lucas Kreuzer[1], Tobias Widmann[1], Nuri Hohn[1], Kun Wang[1], Jean-Francois Moulin[2], Viet Hildebrand[3], André Laschewsky[3], Christine M. Papadakis[1], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]HZG at MLZ, 85747 Garching — [3]Universität Potsdam, Inst. für Chemie, 14476 Potsdam Golm

Responsive polymers can react with a strong change in volume towards even small changes of an external stimulus. This behavior makes them attractive for a manifold selection of applications such as nano-sensors, artificial pumps and muscles or optical switches. In order to implement responsive polymers in the aforementioned application fields, a fundamental understanding of the underlying water kinetics of these polymers is necessary. We follow the water and deuterated water swelling and the corresponding exchange processes in a multi-stimuli responsive block copolymer thin film via in-situ time of flight neutron reflectometry (TOF-NR). The kinetic processes are followed with a high time resolution. The observed swelling and exchange kinetics are modelled to obtain detailed insights about the underlying mechanisms of water uptake and exchange.

CPP 21.8 Tue 11:45 C 130

Swelling Behavior of Thin Hydrogel Films in Humidity and when Water-immersed — •Fabian Muralter and Anna Coclite — Institute of Solid State Physics, TU Graz, Austria

Hydrogels are water-containing networks of hydrophilic polymers, whose distinct properties allow for a number of different applications (e.g. in drug delivery, contact lenses). Their characteristic swelling behavior makes hydrogels particularly interesting for sensor & actuator setups. However, as water diffusivity is the time-limiting step in (de-)swelling, film thickness is crucial for fast response times. In this study, hydrogels are synthesized by initiated Chemical Vapor Deposition (iCVD), with film thicknesses ranging from tens to several hundreds of nanometers. iCVD is a solvent-free technique that allows for precise thickness control and enables a plethora of chemical compositions to be studied. Depending on monomer and crosslinker choice, these hydrogels show different response characteristics depending on the environment (humidity/water immersion). Addition of temperature-sensitive groups such as NIPAAm facilitates also temperature-dependent swelling. The swelling behavior is studied by spectroscopic ellipsometry, which records the evolution of (polymer) optical parameters during swelling as a function of temperature and humidity. This allows for the detection of thickness changes in the Å-range (e.g. thermal expansion) up to full swelling of the hydrogels, with thickness increases of up to 100%. For example, DEAAm-based copolymers show swelling response-times in humidity in the seconds-range, making them highly promising for sensing applications.

CPP 21.9 Tue 12:00 C 130

Transport and solvation of penetrant molecules in a thermoresponsive hydrogel — •Matej Kanduc[1], Won Kyu Kim[1], Rafael Roa[1], and Joachim Dzubiella[1,2] — [1]Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D-14109 Berlin, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany

Thermoresponsive hydrogels have become increasingly interesting materials for pharmaceutical and biomedical applications, primarily due to their high water content and rubbery nature, which is similar to natural tissue, as well as their biocompatibility. External stimuli, such as changes in temperature, trigger the transition from a swollen into a collapsed state of the polymer, which dramatically alters the thermodynamic and transport properties of penetrant molecules. We employ molecular dynamics simulations of a Poly(N-isopropylacrylamide) (PNIPAM) hydrogel with explicit water in its collapsed as well as in the swollen state. The simulations enable us to gain insights into the diffusion and solvation mechanisms of various penetrant molecules in the hydrogel. We find that formations of water pockets, the presence of crosslinkers in the hydrogel, and the polarity of the molecules play a detrimental role for the diffusion mechanisms and solvation free energies. Finally, we discuss how can the observed phenomena be exploited in hydrogel-based applications of responsive nanoreactors for nanocatalysis.

CPP 21.10 Tue 12:15 C 130

Water uptake and diffusion in thin PNIPAM microgel films — •Tobias Widmann[1], Lucas Kreuzer[1], Nuri Hohn[1], Lorenz Biessmann[1], Kun Wang[1], Jean-François Moulin[2], Yvonne Hertle[3], Thomas Hellweg[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]HZG at MLZ, 85747 Garching — [3]Universität Bielefeld, Fakultät für Chemie, Physikalische und Biophysikalische Chemie III, 33615 Bielefeld

Microgels out of thermoresponsive polymers show a strong change in volume by a variation of the temperature across the lower critical solution temperature (LCST), which in a thin film geometry translates into a change of the film thickness. This offers new functionality and is of high interest e.g. for biomedical applications. In order to gain detailed insights in the kinetics during the volume change, the diffusion of water molecules through the interconnected polymer network during the uptake and release of water is analyzed. Thin PNIPAM microgel films crosslinked with N,N'-methylenebisacrylamide are investigated with time-of-flight neutron reflectometry (TOF-NR). H2O and D2O are used to apply different humidity conditions at a constant temperature below the LCST of PNIPAM. The H2O and D2O swelling as well as the H2O - D2O and D2O - H2O exchange processes are studied. Results from the TOF-NR analysis are modelled with a model which accounts for the temporal evolution of the humidity.

CPP 21.11 Tue 12:30 C 130

Multiscale modeling of multiresponsive smart soft matter — Chathuranga De Silva[1], Porakrit Leophairatana[1], Takahiro Ohkuma[2], Jeffrey Koberstein[1], Kurt Kremer[3], and •Debashish Mukherji[3] — [1]Department of Chemical Engineering, Columbia University, New York USA — [2]Central Research Division, Bridgestone Corporation, Kodaira, Tokyo 187-8531 Japan — [3]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz Germany

Design of multiresponsive smart, soft materials is at the onset of many developments in polymer physics, chemical physics, biophysics and biochemistry research. A system is known as smart responsive when a slight change in external stimuli can drastically alter its structure, function, and stability. Because the properties of these systems are dictated by large conformational/compositional fluctuations, it is very difficult to address these problems within both experimental and theoretical setups. On such system is the acetal based copolymers, consisting of repeat units of hydrophobic (methylene) and hydrophilic (ethylene oxide) monomers [1]. In this context, polymer properties are inherently multiscale in nature, where delicate local interaction details play a key role in describing their global conformational behavior. In this presentation, we will discuss the recently developed segment-based multiscale model of these polymers [2]. Furthermore, we will show how our approach can be used to interpreting and guiding experiment towards new directions. [1] Samanta, Bogdanowicz, Lu, and Koberstein, Macromolecules 49, 1858 (2016). [2] De Silva, Leophairatana, Ohkuma, Koberstein, Kremer, and Mukherji, JCP 147, 064904 (2017).

CPP 21.12 Tue 12:45 C 130

Crosslinking Effect on Solute Adsorption in Swollen Thermoresponsive Hydrogels — •Sebastian Milster[1,2], Richard Chudoba[1], Matej Kanduc[1], and Joachim Dzubiella[1,2] — [1]Helmholtz-Zentrum Berlin — [2]Humboldt-Universität zu Berlin

Polymeric networks of poly(N-isopropylacrylamide) (PNIPAM) and N,N'-methylenebisacrylamide crosslinkers (BIS/MBA) are used for tailoring thermoresponsive hydrogels, which exhibit a sudden, yet reversible collapse when exceeding a critical temperature (LCST) of approximately 305K. Along with the volume change, selective solute permeability and adsorption in the gel also undergo a transition. This yields great potential for many applications in which controlled release or uptake of solutes is required. In this work we investigate the impact of crosslinking on solute adsorption in the swollen hydrogel by means of classical molecular dynamics (MD) at 290K. We perform all-atom, explicit water simulations of representative hydrogel subunits in the crosslinker vicinity. The studied system consists of one BIS-linker with four atactic PNIPAM 12-mers in a tetrahedral setup. The interaction between the polymer and cosolutes such as ions, alkanes and aromatics is examined by analysing the radial distribution function. We observe that the solute-specific binding known from single chains[1] is magnified, which should be considered in future hydrogel modeling.

[1] Matej Kanduč et al. "Selective solute adsorption and partitioning around single PNIPAM chains" PCCP 19.8 (2017).

CPP 22: Data-driven Methods in Molecular Simulations of Soft-Matter Systems

Time: Tuesday 9:30–10:30 Location: C 230

CPP 22.1 Tue 9:30 C 230

Consistent interpretation of protein simulation kinetics using Markov state models biased with external information — •Joseph Rudzinski, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz

Molecular simulation models are often required to provide a microscopically-detailed interpretation of observations from, e.g., single-molecule spectroscopy experiments of proteins. In general, model errors may lead to inconsistencies between simulated and experimentally-measured observables. For static properties, well-established reweighting methods exist for adjusting the simulated ensemble with minimum bias in order to attain consistency for observables of interest. This work presents an analogous reweighting framework that adjusts the ensemble of dynamical paths sampled in a molecular simulation in order to ensure consistency with kinetic observables. The proposed methodology leverages Markov state modeling techniques to efficiently treat the simulated dynamical paths, while employing a Bayesian scheme to reweight these paths with minimum bias according to external reference data. Using small peptide systems as a proof of concept, we demonstrate how biasing a Markov state model significantly improves the kinetic description of the system, while refining the static equilibrium properties. Our conclusions highlight the potential of the methodology for providing consistent interpretations of kinetic protein experiments.

CPP 22.2 Tue 9:45 C 230

A complete map between amphiphilic sequences and polymer transport through biological barriers: A massively parallel Rosenbluth study. — •Marco Werner[1], Yachong Guo[2], and Vladimir Baulin[1] — [1]Universitat Rovira i Virgili, Tarragona, Spain — [2]National Laboratory of Solid State Microstructure, Department of Physics, Nanjing University, China

We investigate the relation between the monomer sequence of a polymer composed from hydrophilic and hydrophobic units and its diffusive transport through a lipid membrane. We employ the Rosenbluth method in order to generate random polymer conformations within a given mean fueld potential that represents a membrane or more complex morphologies. Thanks to the massively parallel generation of 1.5×10^7 independent conformations per sequence on graphics processing units (GPU), we obtain the free energy of the polymer with respect to a given reaction coordinate for all sequence combinations with a length $N \leq 16$ in reasonable time. For the prototypical example of the passive transport of polymers through lipid membranes, our results confirm earlier predictions that an overall balance of hydrophilic / hydrophobic units as well as sequences with short blocks lead to a minimal first escape time of the polymer through the membrane.

CPP 22.3 Tue 10:00 C 230

Multiscale approach to conformational sampling: solute insertion in a lipid membrane — •Roberto Menichetti, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

The accurate determination of the thermodynamic properties of soft matter by means of classical atomistic molecular dynamics simulations is often hampered by sampling issues. Coarse-grained models, which describe the system at a lower resolution, provide an efficient tool for addressing this problem. Indeed, coarse-graining smoothens the rough atomistic energy (and consequently free-energy) landscape, thus reducing some of the difficulties of an adequate conformational sampling. In this work, we present a multiscale method which aims at accelerating the exploration of the complex atomistic conformational space by leveraging the one generated by coarse-grained simulations, and apply it to the determination of the potential of mean force for the insertion of a small molecule in a lipid membrane environment. The method offers accurate results with a gain in computational time of roughly one order of magnitude with respect to conventional all-atom umbrella sampling simulations. We further show how the method can be efficiently employed in the framework of computational high-throughput drug screening.

R. Menichetti, K. Kremer and T. Bereau, Biochem. Biophys. Res. Commun. (in press), doi: https://doi.org/10.1016/j.bbrc.2017.08.095 (2017).

CPP 22.4 Tue 10:15 C 230

Intermolecular interactions in complex liquid systems studied by MD simulations — •Nebojša Zec[1], Abdenacer Idrissi[2], Slobodan Gadžurić[3], and Milan Vraneš[3] — [1]GEMS at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht, Garching bei München, Germany — [2]Université des Sciences et Technologies de Lille 1, Villeneuve d'Ascq, France — [3]University of Novi Sad, Department of Chemistry, Biochemistry and Environmental Protection, Novi Sad, Serbia

We used molecular dynamics (MD) simulations to quantify the intermolecular interactions in pure molecular solvents (γ-butyrolactone, γ-valerolactone, propylene carbonate) and their binary mixtures with imidazolium based ionic liquids. The intermolecular interaction potentials were adjusted to reproduce the experimentally measured density of the pure substances as well as the mixtures over the whole range of mixing ratios. Hydrogen bonds, dipole-dipole and stacking interactions are the main interactions in these systems. Comparison of the hydrogen bond geometries with literature values indicates clearly that the hydrogen bond interactions in these systems are comparatively weak. Orientational correlations were characterized by several combined angular and distance distribution functions between first neighbour molecules: The position and tilt of the ring planes with respect to each other indicate ring stacking; and the relative orientation of the C=O bonds shows the relative orientation of molecular dipoles.

CPP 23: Organic Photovoltaics I

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

Invited Talk CPP 23.1 Tue 9:30 C 243

Non-fullerene acceptors for commercially viable organic photovoltaics — •Derya Baran — King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia

The commercialization of OPV requires the availability of inexpensive materials in large quantities, such as poly(3-hexylthiophene) (P3HT). P3HT is readily scalable via flow or micro-reactor synthesis, even using green solvents, whilst retaining a high degree of control over molecular weight and regio-regularity. However, it has a limited open-circuit voltage (Voc), short-circuit current (Jsc) and stability in photovoltaic devices when fullerene derivatives are used as acceptors. This talk will focus on the alternative small molecule non-fullerene acceptors that lead to the highest power conversion efficiencies with P3HT donor. The devices show excellent stability in air and are promising for commercializing OPV in the near future.

CPP 23.2 Tue 10:00 C 243

Developing design criteria for organic solar cells using well-absorbing non-fullerene acceptors — •Lisa Krückemeier[1], Pascal Kaienburg[1], and Thomas Kirchartz[1,2] — [1]IEK5 Photovoltaics, Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — [2]Faculty of Engineering and CENIDE, University of Duisburg-Essen, Carl-Benz-Str. 199, 47057 Duisburg, Germany

In recent years, a variety of promising, well-absorbing non-fullerene acceptor molecules (NFAs) for bulk heterojunction OPV has been developed, which often achieve higher efficiencies than their fullerene-based counterparts. Unlike fullerene acceptors, these various NFAs have their respective absorption peak at different positions of the visible spectrum, allowing the absorption behavior of the blend to be flexibly adjusted by changing its composition. Thus, the fundamental question arises, how to adjust these two absorption spectra of the acceptor and donor to each other in order to best exploit the incident power of the sun and get high solar cell efficiencies. A series of parameters, such as layer thickness, electronic quality and the amount of non-radiative voltage losses affects this optimum. By using numerical simulations, we have developed design criteria for organic solar cells with well-absorbing non-fullerene acceptors that take these influences into account. Only when the electronic quality of the layer still allows a sufficient charge carrier collection for layer thicknesses around the second interference maximum, a combination of complementary absorbing molecules is more efficient. For smaller thicknesses, a blend of molecules with the same absorption onset achieves higher efficiencies.

CPP 23.3 Tue 10:15 C 243

Photovoltaic Performance of Non-Fullerene Acceptors with Anthracene-Containing PPE-PPV — Shahidul Alam[1,2], Rico Meitzner[1,2], Christian Friebe[1,2], Jonathan Cann[4], Johannes Ahner[2], Christoph Ulbricht[3], Zhipeng Kan[5], Stephanie Hoeppener[2], Martin D. Hager[1,2], Daniel A. M. Egbe[3], Gregory C. Welch[4], Frédéric Laquai[5], Ulrich S. Schubert[1,2], and •Harald Hoppe[1,2] — [1]CEEC, Friedrich Schiller University Jena — [2]IOMC, Friedrich Schiller University Jena — [3]Institute of Polymeric Materials and Testing, Johannes Kepler University, Linz, Austria — [4]Department of Chemistry, University of Calgary, Canada — [5]KAUST, Kingdom of Saudi Arabia

Recently, non-fullerene acceptors (NFAs) have received increasing attention for use in polymer-based bulk-heterojunction organic solar cells, as they have demonstrated improved photovoltaic performances as compared to conventional polymer-fullerene blends. Polymer solar cells based on an anthracene-containing poly(p-phenylene ethynylene)-alt-poly(p-phenylene vinylene) (PPE*PPV) copolymer with statistical side chain configuration (AnE-PVstat) in combination with various electron accepting materials were prepared and studied. In contrast to blends with PCBM, the almost complete extinction of the polymer photoluminescence in these donor-acceptor blends indicated too fine-scaled intermixing. This seems to cause poor photovoltaic performance. Time-delayed collection-field (TDCF) measurements revealed that the photovoltaic effectiveness of these organic semiconductor blends was strongly limited by insufficient charge generation and extraction.

CPP 23.4 Tue 10:30 C 243

The Impact of Driving Force and Temperature on the Electron Transfer in Donor-Acceptor Blend Systems — T Unger[1], •S Wedler[1], F-J Kahle[1], U Scherf[3], H Bässler[2], and A Köhler[1,2] — [1]Experimental Physics II, Uni Bayreuth — [2]BIMF, Uni Bayreuth — [3]Makromolekulare Chemie, Uni Wuppertal

We discuss whether electron transfer from a photoexcited polymer donor to a fullerene acceptor in an organic solar cell is tractable in terms of Marcus theory, and whether the driving force $\Delta G0$ is crucial in this process (JPCC 2017, 121, 22739). Considering Marcus rates to be thermally activated, we measured the appearance time of the polaron signal between 12 and 295 K for the representative donor polymers PTB7, PCPDTBT and Me-LPPP blended with PCBM. In all cases, the dissociation process was faster than the temporal resolution of our experimental setup (220-400 fs), suggesting that the charge transfer is independent of $\Delta G0$. We find that for the PCPDTBT:PCBM ($\Delta G0=0.2$ eV) and PTB7:PCBM ($\Delta G0=0.3$ eV) the data is mathematically consistent with Marcus theory, yet the condition of thermal equilibrium is not satisfied. For MeLPPP:PCBM in the Marcus inverted regime, the dissociation rate is inconsistent with Marcus theory but formally tractable using the Marcus-Levich-Jortner tunneling formalism which also requires thermal equilibrium. This is inconsistent with the short transfer times we observed and implies that coherent effects need to be considered. Our results imply that any dependence of the total photocurrent yield must be ascribed to the secondary escape of the initially generated CT-state from its Coulomb potential.

CPP 23.5 Tue 10:45 C 243

Charge photogeneration in organic solar cells composed of over 90% C60 — •Elisa Collado-Fregoso[1], Johannes Benduhn[2], Koen Vandewal[2], and Dieter Neher[1] — [1]Institut für Physik und Astronomie, Potsdam University, Karl-Liebknecht-Straße 24-25, 14476 Potsdam-Golm, Germany — [2]Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, Nöthnitzer Str. 61, 01187 Dresden, Germany

The involvement of charge-transfer (CT) states in the processes of charge generation and recombination has been an important focus of study within the organic photovoltaic community. However, it has proved challenging to systematically address specific molecular properties without modifying the microstructure of the blend. In this work, we study the mechanism of charge generation in a series of solar cell devices with active layers composed mainly of vacuum deposited C60 and small amounts (~ 5% mol) of organic molecular donors. This ensures a constant morphology dictated by the fullerene acceptor. Using time-delayed collection field measurements, we demonstrate that the short circuit current and fill factor in these devices are largely determined by the charge generation efficiency and its bias dependence, which is more pronounced with decreasing CT state energy. This finding challenges current views that the existence of fullerene aggregates is sufficient to ensure efficient CT dissociation, and questions the picture of a necessary driving energy for charge generation. We discuss the implications of these findings within the framework of the Onsager-Brown model and propose guidelines to improve charge generation.

15 min. break

CPP 23.6 Tue 11:15 C 243

Phonon-Induced Absorption Line Shapes in Organic Semiconductors — •Michel Panhans[1], Johannes Benduhn[2], Karl Sebastian Schellhammer[1], Koen Vandewal[2], and Frank Ortmann[1] — [1]Center for Advancing Electronics Dresden, TU Dresden — [2]Institute for Applied Photophysics, TU Dresden

Quantifying disorder is an important task in organic semiconductor research [1,2] because of its impact on the carrier mobility and device performance. We analyze models of amorphous and crystalline donor-acceptor systems regarding their response to optical excitations. [3] We study the excited-state density of states with varying electronic disorder and electron-phonon interaction and compare our results to absorption measurements on donor-acceptor blends.

[1] D. Venkateshvaran et al. Nature 515, 384 (2014).

[2] K. Vandewal et al. J. Am. Chem. Soc. 139, 1699 (2017).

[3] M. Panhans et al. (in preparation)

CPP 23.7 Tue 11:30 C 243

Investigation of degradation processes in low bandgap polymers for organic photovoltaics — •Franziska C. Löhrer, Christoph Senfter, and Peter Müller-Buschbaum — TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organic photovoltaics have experienced a drastic increase in research and are gaining impact as a feasible alternative to conventional solar cells. With their easy processability, high flexibility and tunable optical properties, organic materials such as photoactive polymers offer a wide range of potential applications. Recent efforts focus on identifying new materials in order to enhance the device performance. This has led to the development of low bandgap polymers such as PTB7 and its derivatives with reported efficiencies surpassing the 10 % limit. However, especially high-efficiency polymers are sensitive to various degradation processes, which strongly decrease their lifetime. We follow the chemical and physical changes occurring inlow bandgap polymers during light-induced aging and test ways to eliminate typical degradation pathways. The thin film morphology is investigated using real-space imaging as well as X-ray scattering techniques. Optical and IR spectroscopy methods give insights into the chemical changes inside the polymer.

CPP 23.8 Tue 11:45 C 243

Charge Carrier Recombination Dynamics in Squaraine-Based Bulk-Heterojunction Solar Cells — •Dorothea Scheunemann[1], Oliver Kolloge[1], Sebastian Wilken[1], Majvor Mack[1], Jürgen Parisi[1], Matthias Schulz[2], Arne Lützen[2], and Manuela Schiek[1] — [1]University of Oldenburg, Institute of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg — [2]University of Bonn, Kekulé Institute of Organic Chemistry and Biochemistry, 53121 Bonn

Squaraine (SQ) dyes receive increasing attention as donor materials in organic photovoltaics since they combine high absorption in the deepred with a general environmental stability and non-toxicity. Together with common fullerene acceptors, SQ-based bulk-heterojunction devices have been demonstrated to deliver a high open-circuit voltage, but suffer from a comparatively low fill factor [1]. However, little effort has been made to develop a better understanding of the underlying loss mechanisms. In this work, we focus on transient optoelectronic characterization methods to study the loss mechanisms in photovoltaic devices of a benchmark squaraine (SQIB) blended with a fullerene (PC60BM). These devices show a gradual decrease of the fill factor when increasing the active layer thickness and incident light intensity. We show that the low fill factor is a consequence of slow charge carrier collection competing with bimolecular recombination.

[1] Scheunemann et al., Appl. Phys. Lett. 111 (2017) 183502.

CPP 23.9 Tue 12:00 C 243

Recombination in Organic Solar Cells: Are There Still Lessons to Learn from P3HT:PCBM? — •Sebastian Wilken, Dorothea Scheunemann, and Jürgen Parisi — Institute of Physics, University of Oldenburg, Germany

The nature of the non-geminate recombination in organic bulk heterojunction solar cells remains controversial. In this talk, we present new data on an old hat: P3HT:PCBM. By tailoring the nanoscale morphology, we observed a novel kind of structure–property relationship in P3HT:PCBM devices that is at variance with current theoretical models. We discuss whether these findings provide new avenues for understanding the role of phase separation and interface states in the non-geminate recombination dynamics.

CPP 23.10 Tue 12:15 C 243

Apparent Field Dependence of Charge Carrier Generation and Recombination Coefficient in Organic Solar Cells — •Uli Würfel and Moritz Unmüssig — Fraunhofer ISE, Heidenhofstr. 2, 79110 Freiburg, Germany

Charge carrier generation in organic solar cells is often reported to show an electric field dependence. However, it is not measured directly but is derived from transient charge carrier extraction experiments based on the time delayed collection field (TDCF) method. In this contribution, numerical simulations of TDCF experiments are presented which - when analyzed in the same way as reported in literature - result in a field dependence of the charge carrier generation and the recombination coefficient even though field-independent values are used. For the carrier generation this discrepancy is consistently shown to be caused by (unavoidable) bi-molecular recombination in the short time scale prior to and during extraction. The apparent field dependency becomes more pronounced with increasing recombination coefficient and decreasing charge carrier mobilities, well in accordance with TDCF data from literature. The apparent field dependence of the bimolecular recombination coefficient is due to the fact that its derivation from experimental TDCF data is based on spatially averaged values of carrier densities. In contrast, electrons and holes in real devices are distributed inhomogeneously as a consequence of the boundary conditions. Our study shows clearly that in order to explain results from TDCF experiments it is not required to include any field-dependence nor of the photocurrent generation nor of the recombination coefficient.

CPP 23.11 Tue 12:30 C 243

Effect of the RC time on photocurrent transients and determination of charge carrier mobilities — •Juliane Kniepert and Dieter Neher — University of Potsdam, Germany

We present a closed analytic model to describe time dependent photocurrents upon pulsed illumination in the presence of an external RC circuit. In combination with numerical drift diffusion simulations, it is shown that the RC time has a severe influence on the shape of the transients. In particular, the maximum of the photocurrent is delayed due to a delayed recharging of the electrodes. This delay increases with increasing RC constant. As a consequence, charge carrier mobilities determined from simple extrapolation of the initial photocurrent decay will be in general too small and feature a false dependence on the electric field. Here, we present a recipe to correct charge carrier mobilities determined from measured photocurrent transients by taking into account the RC time of the experimental set-up. We also demonstrate how the model can be used to more reliably determine the charge carrier mobility from experimental data of a typical polymer/fullerene organic solar cell. It is shown that further aspects like a finite rising time of the pulse generator and the current contribution of the slower charger carriers influence the shape of the transients and may lead to an additional underestimation of the transit time.[1]

[1] Kniepert et al., J. Appl. Phys. 122, 195501 (2017)

CPP 23.12 Tue 12:45 C 243

Parameter extraction from measured solar cell IV curves using CELIC model — •Vladislav Jovanov, Arne Müller, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Current voltage (IV) characteristic of solar cells with low mobility of charge carriers cannot be described using classical Shockley model. To properly describe behavior of low-mobility solar cells, we have developed analytical CELIC model based on simplified drift-diffusion calculations [1]. This model assumes a constant electric field (CE) and linearly increasing current (LIC) contributions of holes an electrons inside the semiconductor layer. Furthermore, the developed model takes into account recombination processes within the semiconductor bulk and at the contact interfaces. We have already shown that CELIC model is not limited only to solar cells with low mobility of charge carrier, and it can be also used for modeling of perovskite and silicon solar cells. In this study, we show how to extract material parameters from measured solar cell IV curves using CELIC model. For this purpose, we have fabricated organic bulk hetero-junction solar cells for different composition ratio of polymer and fullerene using solution processing. By applying CELIC model, we can analyze the crossing point between dark and light curves and access mobility and contact properties in dependence of composition of the semiconductor layer.

[1] A.Müller, V.Jovanov, V.Wagner, Appl.Phys.Lett. 111 (2017) 023506

CPP 24: Complex Fluids and Colloids II (joint session CPP/DY)

Time: Tuesday 9:30–11:45 Location: C 264

CPP 24.1 Tue 9:30 C 264

Effective Landau description of ferronematics — •Grigorii Zarubin[1,2], Markus Bier[1,2], and Siegfried Dietrich[1,2] — [1]Max Planck Institute Int. Sys. — [2]University of Stuttgart, Germany

A ferromagnetic phase of anisotropic particles suspended in a nematic liquid crystal (NLC) was predicted as early as 1970 [1]. A recent experimental realization [2] confirmed that a dilute suspension of magnetic platelets in NLC forms ferromagnetic phase which is susceptible to weak magnetic fields. In this work we develop a Landau-like description of such a suspension starting from a microscopic model. Our functional represents an expansion in powers of two spatially varying fields: i) magnetization field and ii) director field and their cross terms. Using this result we can compare our theory to the one proposed in [2], in particular we have an access to the effective coupling coefficient between magnetization and director field which provides a way to estimate coupling of the director to the surface of the single platelet experimentally.

[1] F. Brochard and P.G. de Gennes, J. Physique 31, 691 (1970).

[2] A. Mertelj, D. Lisjak, M. Drofenik and M. Copic, Nature 504, 237 (2013).

CPP 24.2 Tue 9:45 C 264

Self-assembly of colloidal particles with a magnetic coating under external magnetic fields — Gabi Steinbach[1,2], Michael Schreiber[1], Dennis Nissen[3], Manfred Albrecht[3], •Ekaterina Novak[4], Pedro A. Sanchez[5], Sofia Kantorovich[4,5], Sibylle Gemming[1,2], and Artur Erbe[2] — [1]Institute of Physics, Technische Universität Chemnitz, 09107 Chemnitz, Germany — [2]Lenin Av.51 — [3]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany — [4]Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia — [5]Computational Physics, Universität Wien, Sensengasse 8, Vienna, 1090, Austria

In recent years, in order to build tailored structures, magnetic nanoparticles and colloids that deviate from the model of a spherical particle with a dipole moment at its center were studied. Among them are dumbbells, magnetic core-shell particles, elongated ferroparticles, and colloidal particles with a magnetic cap. In this contribution, we both experimentally and numerically shows how an equilibrium state with non-collinear arrangement of the magnetic moments of colloidal particles with a magnetic cap enables the controlled self-assembly of diverse structures in two dimensions via constant and low-frequency external magnetic fields. Branched clusters of staggered chains, compact clusters, linear chains, and dispersed single particles can be formed and interconverted. The presented precise control of structure formation and reconfiguration under external fields of only a few mT open new potential for using in responsive materials for highly sensitive magnetic and optical applications.

CPP 24.3 Tue 10:00 C 264

Self-assembly of magnetic filaments with different topologies — •Elena Pyanzina[1], Ekaterina Novak[1], Dmitry Rozhkov[1], Pedro Sanchez[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

Semi-flexible polymer-like chains of magnetic nanoparticles permanently crosslinked with polymers (magnetic filaments) have been recently pointed as promising building blocks for the creation of sophisticated magnetoresponsive materials. Our research addresses the study of magnetic filaments with different chain conformations - simple open chains, closed rings and branched structures with "X" and "Y" junctions - inspired by the recent findings on the low temperature self-assembly of dipolar hard spheres (Kantorovich et al, PCCP, 2015). The introduction of the polymer crosslinkers to stabilise the structure of such self-assembled nanoparticle aggregates is expected to have an important impact on the properties of the system. Here we focus on low-concentration solutions, analysing in detail their self-assembly behaviour. Extensive cluster analysis allows us to compare the structures formed by these filament solutions to those observed in "conventional" magnetic fluids containing non-crosslinked nanoparticles. These results will pave the way for the development of analytical models and identify the most interesting building block candidates for the design of novel magnetoresponsive materials.

CPP 24.4 Tue 10:15 C 264

Magnetic microgels in computer simulations — •Elena Minina[1,2], Pedro Sanchez[1], Christos Likos[1], and Sofia Kantorovich[1,2] — [1]University of Vienna, Vienna, Austria — [2]Ural Federal University, Ekaterinburg, Russian Federation

In this work, we study magnetic microgels – spherical colloidal particles consisting of polymer network with embedded magnetic dipolar particles – by means of molecular dynamics computer simulations. Our main focus is concentrated on how the microgels change their shape and size depending on their internal structure and magnetic component. Microgels are initially modelled as bead-spring polymer chains randomly crosslinked into a polymer network. Changing degree of crosslinking allows us to vary microgel's internal structure. This way, we consider weekly crosslinked and highly crosslinked microgels. The fraction of magnetic particles is in the range between 0.5 to 10 per cent of the total fraction of particles comprising the polymer network. Studying such systems at different strength of dipole-dipole interactions, we estimate the change of magnetic microgel in size, self-assembly of magnetic particles and the initial magnetic susceptibility. We show that an appropriate combination of magnetic component and degree of crosslinking may offer an additional way to control.

CPP 24.5 Tue 10:30 C 264

Influence of rotating magnetic field on magnetic fluids with different viscosities — •Anastasia Storozhenko[1], Ralf Stannarius[2], Alexey Eremin[2], Torsten Trittel[2], and Igor Aref'ev[3] — [1]Southwest State University, 305040 Kursk, Russia — [2]Otto von Guericke University Magdeburg, 39016 Magdeburg, Germany — [3]Ivanovo Power Engineering University, 153003, Ivanovo, Russia

In an external rotating magnetic field, the magnetization of magnetic nanoparticles follows the field direction with a certain phase lag, which results in a macroscopic torque. We investigated experimentally the dependence of the torque density on the strength and frequency of the magnetic field, as well as on the viscosity of magnetic fluid.

The torque density increases with the square of the field strength; this can be explained by well-known expressions. At the same time, the magnetization direction changes slower than the external magnetic field due to the relaxation of magnetic nanoparticles. The dependence of the torque on frequency is thus complex and depends on the viscosity of magnetic fluid. We find a growth of the torque with rotation rate of the field, followed by a decay at higher rates. The torque maximum shifts with changing viscosity. This phenomenon can be related to the balance of Neel and Debye relaxation times.

This study was funded by DFG within SPP 1681, Project STA 425/36 and a DAAD Stipendium.

CPP 24.6 Tue 10:45 C 264

Microfludic-SANS: Rapid screening and flow processing of complex fluids — •Carlos Lopez[1], Takaichi Watanabe[2], Marco Adamo[3], Andreas Poulos[3], Anne Martel[4], Lionel Porcar[4], and Joao Cabral[3] — [1]RWTH Aachen University — [2]Okayama University — [3]Imperial College London — [4]Institut Laue Langevin

The coupling of microfluidics and small angle neutron scattering (SANS) is demonstrated. We have developed microfluidic devices with low SANS background and high pressure resistance for the investigation of flow-induced phenomena and high throughput phase mapping of soft matter.

We study the structure of model water-surfactant-oil mixtures under extensional flow and obtain scattering profiles from 50 micron wide channels, with 1 - 300 second acquisition times. The microfluidic geometry enables the variation of both flow type and magnitude, beyond traditional rheo-SANS setups, and is well-suited for complex fluids due to the commensurability of relevant time and lengthscales.

Using an online micromixer we implement a high-throughput approach, scanning in excess of 10 SANS profiles per minute for model surfactant and colloid solutions both in continuous and multiphase (droplet) flow. We show that microfluidic approaches can reduce experimental time and sample volume and considerably improve the accuracy of contrast matching experiments.

15 min. break

CPP 24.7 Tue 11:15 C 264

Biaxial Phases in binary mixtures of liquid crystals — •Robert Skutnik, Louis Lehmann, Sergej Püschel-Schlotthauer, and Martin Schoen — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Sekr. C7, Straße des 17. Juni 135, Berlin 10623, Germany

Liquid crystals are organic molecules of anisotropic shape exhibiting anisotropic interactions. In fact, because of their delocalized π electron system, they exhibit π-π stacking and align parallel with their neighbors. Generally speaking, liquid crystal molecules can be classified as prolate or oblate molecules where the π-π electrons are parallel and perpendicular to the molecular symmetry axis. Hence, the interaction of an oblate and prolate liquid crystal results in a perpendicular alignment with respect to their symmetry axes. We perform Monte Carlo simulations and model both species (i. e., prolate and oblate) by an anisotropic potential based on the well-known 12-6 Lennard-Jones potential which promotes a parallel alignment if both particles are of the same species and perpendicular alignment otherwise. Besides the isotropic phase, we observe the formation of a nematic phase in the presence of a biaxial isotropic phase and the formation of a biaxial nematic phase despite the otherwise uniaxial symmetry of molecules of both species.

CPP 24.8 Tue 11:30 C 264

Polar and nematic liquid crystals on curved surface — •Axel Voigt, Simon Praetorius, Michael Nestler, Ingo Nitschke, and Sebastian Reuther — TU Dresden, Institut für Wissenschaftliches Rechnen

We consider a thin film limit of a Frank-Oseen and a Landau-de Gennes model. In the limiting process we observe a continuous transition where the normal and tangential parts of the director and the Q-tensor decouple and various intrinsic and extrinsic contributions emerge. For the derived surface models, we consider an L^2-gradient flow. The resulting vector- or tensor-valued surface partial differential equations are numerically solved to demonstrate realizations of the tight coupling of elastic and bulk free energy with geometric properties. We further discuss extensions towards surface Ericksen-Leslie and Beris-Edwards models and active liquid crystals on curved surfaces.

CPP 25: Interfaces and Thin Films II

Time: Tuesday 9:30–13:00 Location: PC 203

Invited Talk CPP 25.1 Tue 9:30 PC 203
Understanding self-assembly in gyroid terpolymer films — •Ilja Gunkel — Adolphe Merkle Insitute, Fribourg, Switzerland

Block copolymer (BCP) self-assembly is an effective tool for generating various nanostructured morphologies. Over the past decades, tremendous progress has been made in both understanding and controlling the self-assembly of BCP thin films. However, this has been mostly seen in diblocks, the simplest BCP architecture, enabling the generation of well-ordered two-dimensional patterns with applications, for example, as nanolithography masks. Simply extending a diblock by a third chemically distinct block, thereby creating a so-called triblock terpolymer, provides access to more complex morphologies, *e.g.* the gyroid. The unique geometry of the gyroid - a bicontinuous and triply periodic cubic morphology with inherent chirality - holds promise for enabling new applications like optical metamaterials. Creating the desired functionality in these plasmonic materials requires precise structural control of the polymer template used for their fabrication. However, this level of control and detailed understanding of triblock terpolymer self-assembly have yet to be achieved. In this talk, I will present recent results showing that gyroid terpolymer films with long-range order can be generated by controlled solvent vapor annealing. I will further show that terpolymer self-assembly in films during annealing can be tracked by *in situ* grazing-incidence small-angle x-ray scattering (GISAXS). These experiments provide detailed structural information, which is key to generating well-ordered gyroid terpolymer films that can serve as templates for the fabrication of optical metamaterials.

CPP 25.2 Tue 10:00 PC 203
Solvothermal Annealing of a Diblock Copolymer Film in Solvent Vapor Mixtures — Anatoly V. Berezkin[1], Florian Jung[1], Dorthe Posselt[2], Detlef-M. Smilgies[3], and •Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Roskilde University, Department of Science and Environment, Denmark — [3]Cornell University, Cornell High Energy Synchrotron Source, Ithaca NY, U.S.A.

Solvent vapor annealing is often used to control the structure of block copolymer thin films [1]. Solvothermal vapor annealing (STVA) combined with variable mixing of solvent vapors allows one to produce a number of morphologies. We carried out STVA on a thin film from polystyrene-*b*-polydimethylsiloxane (PS-*b*-PDMS) using vapors from *n*-heptane and toluene at elevated temperature, varying the vapor composition step by step. Cylindrical and lamellar morphologies are detected using *in-situ*, real-time grazing-incidence small-angle X-ray scattering. To corroborate these morphologies, they are generated by molecular simulations, and the corresponding 2D GISAXS maps are calculated. The solvent distribution in the two types of nanodomains is estimated from the intensity of the Bragg reflections along with the swelling ratio of the film. The combination of these methods opens up for the efficient preparation of block copolymer thin films having the desired morphology and orientation and furthers the understanding of the underlying mechanisms.

[1] Posselt et al., *Prog. Polym. Sci.* **66**, 80 (2017).

CPP 25.3 Tue 10:15 PC 203
Self-propulsion of Janus Particles near a brush Surface: Impact of the Brush Chain Length — •Mojdeh Heidari[1], Santiago Muinos Landin[2], Frank Cichos[2], and Regine von Klitzing[1] — [1]Smart Matter at Interfaces, Department of Physics, Technical University of Darmstadt, Alarich-weiß-straße 10, 64287 Darmstadt, Germany — [2]Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Faculty of Physics and Earth Sciences, Universität Leipzig, Linnéstraße 5, 04103 Leipzig, Germany

GoldAu-polystyrene Janus particles demonstrate a thermophoretic induced motion under laser illumination (λ=532 nm). The plasmons in the gold cap of the particle get excited and cause the particle to create a local temperature gradient. Such out-of-equilibrium condition at the surface of the particle leads to its self-propulsion.

In this study we explore the 2D self-propulsion of Janus particles between two glass substrates. The substrate is functionalized with PNIPAM brushes. Our former experiments have proved that particles express an enhanced self-propulsion close to PNIPAM-brush. Here we alter the brush thickness and subsequently investigate its impact on the self-propulsion of the particle. Trajectories of particles are represented under different laser intensities.

CPP 25.4 Tue 10:30 PC 203
Near surface dynamics of PEG and PNIPAM based polymer brushes — •Judith Witte[1], Tetyana Kyrey[1,2], Regine von Klitzing[3], Olaf Holderer[2], and Stefan Wellert[1] — [1]TU Berlin, Institute for Chemistry, Berlin, Germany — [2]Heinz Maier Leibniz Zentrum, JCNS, Garching, Germany — [3]TU Darmstadt, Institute for Condensed Matter Physics, Darmstadt, Germany

The physical properties of stimuli-responsive polymer brushes still receive vast interest in basic research. Polymer brushes undergoing a temperature induced phase transition are of major interest for technical applications such as (bio)functional coatings. Polymer brushes are polymers end-tethered to a solid surface. A variation of the chemical composition, brush height or grafting density allows for a wide range of different polymer coatings with distinct properties. Among them, thermoresponsive polymer brushes based on P(MEO$_2$MA-co-OEGMA) are, due to their biocompatibility, promising candidates for smart biocoatings. PNIPAM based polymer brushes serve as a prominent model system for thermoresponsive polymer coatings. Here we focus on recent grazing incidence neutron spin echo spectroscopy experiments probing the dynamics inside these polymer brush layers on the nanometer length and nanosecond time scale. At two neutron penetration depths we explored the segmental dynamics well below the LCST. The data suggest an influence of the nonuniform blob size on the relaxation time inside the brushes which is discussed in the talk.

CPP 25.5 Tue 10:45 PC 203
3D Depth Profiles of the Tip-Sample Interaction on Polystyrene Swollen in Chloroform Vapor using Atomic Force Microscopy — •Martin Dehnert and Robert Magerle — Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany

In atomic force microscopy (AFM) on soft polymers and liquids, the tip-sample interaction is dominated by long range van der Waals and capillary forces and the tip can indent several tens of nanometers into the surface. Therefore, measuring the unperturbed shape of the soft surface can be challenging. Here, we examine polystyrene droplets swollen in chloroform vapor, where we can adjust the specimens' mechanical properties via the solvent vapor concentration from a stiff solid to a fluid film. With the same AFM tip, we measure three-dimensional (3D) depth profiles of the tip-sample interaction with two different AFM force spectroscopy methods: force-distance (FD) curves and amplitude-phase-distance (APD) curves. The 3D depth profiles reconstructed from FD and APD measurements provide a detailed insight into the tip-sample interaction mechanism with a fluid PS droplet. Furthermore, we discuss how the unperturbed shape of a fluid droplet can be determined from FD and APD depth profiles. We expect that this versatile methodology can also be used for investigating other fluid and gel-like objects on the nanometer scale.

15 min. break

Invited Talk CPP 25.6 Tue 11:15 PC 203
Soft Interfaces Studied with the Quartz Crystal Microbalance — •Diethelm Johannsmann and Arne Langhoff — Institute of Physical Chemistry, TU Clausthal

The response of soft interfaces to acoustic shear waves gives clues to their structure, dynamics, and functionality. This response is conveniently probed with the quartz crystal microbalance (QCM). In recent years, the quartz crystal microbalance has turned into a surface-analytical tool with capabilities much beyond gravimetry.

Among the recent novel application of the QCM is high-frequency contact mechanics. Exploiting the amplitude dependence of the shifts in resonance frequencies and the resonance bandwidths on the different overtones, one can follow the transition from stick to (oscillatory) slip. A second field with recent progress are fast measurements (10 ms) combined with a modulation of the electrical potential. For repetitive processes, accumulation drives the precision down the level of a few mHz. Combination of the QCM with potential modulation amounts to a novel sensing dimension even outside electrochemistry.

CPP 25.7 Tue 11:45 PC 203

Interaction-dependent structure of biomimetic soft interfaces : a new method for neutron reflectometry studies — •Samantha Micciulla[1,2], Yuri Gerelli[2], and Emanuel Schneck[1] — [1]Max-Planck-Institut für Kolloid und Grenzflächenforschung, Potsdam, Germany — [2]Institut Laue-Langevin, Grenoble, France

The structural investigation of biological interfaces encounters significant methodological restrictions, due to the limited number of techniques able to probe buried interfaces with high resolution and in a perturbation-free manner. Neutron reflectometry meets these fundamental requirements and it owes the unique capability of selecting individual parts of molecular assemblies by isotopic labelling. In our group, we exploit this technique to study biomimetic interfaces under controlled interaction conditions. In this contribution, a new method to study the structure of soft interacting surfaces at varying separation distances by neutron reflectometry is presented. The method exploits a fine control of the interfacial distance by moving a lipid monolayer at the oil/water interface against a functionalized solid surface. Its applicability to study interacting soft interfaces is demonstrated by the results of recent experiments on systems showing very diverse interaction behavior, from full adhesion to strong repulsion. Finally, morphological features and dynamics of the fluid interface at different distances from the solid substrate are deduced by fluorescence microscopy.

CPP 25.8 Tue 12:00 PC 203

In situ growth study during spray deposition of bio-based materials — •Calvin Brett[1,2,3], Nitesh Mittal[1,2], Wiebke Ohm[3], Björn Fricke[3], Daniel Söderberg[1], and Stephan V. Roth[3,4] — [1]Department of Mechanics, Royal Institute of Technology (KTH), Stockholm, Sweden — [2]Wallenberg Wood Science Center (WWSC), Stockholm, Sweden — [3]Photon Science, Deutsches Elektronen-Synchroton (DESY), Hamburg, Germany — [4]Department of Fibre and Polymer Technology, Royal Institute of Technology (KTH), Stockholm, Sweden

Assemblies of high aspect-rate nanoparticles are used in large-scale processes to create high-performance materials. We transferred these concepts to self-assembled thin films with tunable properties. Airbrush spray deposition - a scalable and rapid film fabrication process - is used to fabricate cellulose nanofibril (CNF) thin films. CNF as produced from wood presents a renewable and sustainable bio-material which draws increasing attention as template material for flexible, yet disposable electronics. By combining airbrush spray deposition with bio-based materials as CNFs we thus aim for scalable, industrially applicable, sustainable templates. In order to fully understand the fabrication kinetics during film growth, we took the advantage of surface sensitive X-ray scattering techniques in combination with in situ surface differential reflectance spectroscopy. Our study reveals very homogeneous CNF thin films with an unprecedented roughness below 2 nm in combination with a tunable wettability.

CPP 25.9 Tue 12:15 PC 203

Thin films of perflourinated sexithiophene and blends with sexithiophene — •Berthold Reisz[1], Simon Weimer[1], Rupak Banerjee[2], Clemens Zeiser[1], Christopher Lorch[1], Giuliano Duva[1], Johannes Dieterle[1], Keiichirou Yonezawa[3], Jin-Peng Yang[3], Nobuo Ueno[3], Satoshi Kera[3,4], Alexander Hinderhofer[1], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Universität, Tübingen, Deutschland — [2]IIT, Gandhinagar, India — [3]Chiba University, Chiba, Japan — [4]Institute for Molecular Science, Okazaki, Japan

This is the first study of thin films containing perfluorinated sexithiophene (PF6T), a molecule which was firstly synthesized in 2001 [1]. We found a new thin film polymorph and a coexistence of lying-down and standing-up molecules depending on the substrate temperature during organic molecular beam deposition [2]. Furthermore, we prepared blended thin films by co-evaporation of PF6T and its non-fluorinated counterpart 6T at different mixing ratios and examined their morphology, as well as their electronic and optical properties [2]. Atomic force microscopy shows a continuous transition from terraced islands to tall columnar features with increasing amount of PF6T. Grazing incidence X-ray diffraction patterns indicate that an excess of 6T-molecules is segregated from a statistically mixed phase. Finally, UPS data and optical absorption measurements suggest that 6T-PF6T blends could serve as a donor-acceptor system for optoelectronic applications.

[1] Y. Sakamoto et al., J. Am. Chem. Soc. **123** (2001)

[2] B. Reisz et al., J. Mater. Res. **32** (2017)

CPP 25.10 Tue 12:30 PC 203

Real-Time Study on Growth and Packing Behavior of PDIs Thin Films Influenced by Side-Chains Modification — •Valentina Belova[1], Benjamin Wagner[1], Berthold Reisz[1], Clemens Zeiser[1], Giuliano Duva[1], Jakub Rozbořil[2], Jiří Novák[2], Alexander Gerlach[1], Alexander Hinderhofer[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Tübingen, Germany — [2]Masaryk University, Brno, Czech Republic

We study the growth of two highly performing small molecule organic semiconductors from the perylene diimide family (PDIs) interesting for photovoltaic application due to their good electron-accepting properties [1]: PDIR-CN2 and PDIF-CN2 whose chemical structures differ only in the imide substituents: branched alkyl chains and linear fluoroalkyl chains, respectively. Both types of substituents introduce some degree of steric hindrance for intermolecular interaction affecting solid state packing during vacuum deposition and thus induce specific structure-dependent optoelectronic properties in thin films. The phase transition from an amorphous structure to crystalline domains was followed in situ and in real-time by X-ray diffraction as a function of substrate temperature. We examined the relationship between structural properties and optical signatures probed via differential reflectance spectroscopy in real-time, ellipsometry and photoluminescence. A new crystalline polymorph for PDIR-CN2 at high temperatures was found. We observed that the fluorinated chains contribute to crystallization inhibition and surface roughening due to their high electron density. [1] V. Belova et al., JACS, 139, 8474 (2017).

CPP 25.11 Tue 12:45 PC 203

Grazing Incidence Small Angle X-ray Scattering Study on Nucleation Processes during Electrodeposition — •Gilles Moehl and Andrew Hector — Chemistry, University of Southampton, Southampton, SO17 1BJ, UK

Developing the next generation of electronic devices requires the deposition of high-quality functional materials in a controlled fashion in complex structures in order to unleash the true potential of devices such as thermoelectrics, phase change memory (PCM) and infra-red detectors. Within EPSRC programme grant ADEPT *Advanced Devices by ElectroPlaTing* (EP/N035437/1), new techniques and materials are to be developed for that matter. Previously, it has been shown that the electrodeposition of materials from weakly-coordinating solvents is capable of producing such complex structures (1). Nucleation, being the earliest stage of any deposition process is a key feature which has to be understood in order to achieve fully controlled and reproducibly fabricated materials. This requires techniques capable of monitoring the formation of deposited material on a substrate at various stages in time on very short length scales. Grazing incidence small angle scattering (GISAXS) allows for this, giving insight into the structural properties of the investigated layer and thus possibly enables the derivation of a growth model. In this work, the nucleation of the thermoelectric bismuth telluride Bi2Te3 and gold during electrodeposition from dichloromethane and an aqueous electrolyte, respectively, onto titanium nitride (TiN) is investigated through GISAXS. (1).Bartlett, Philip N., et al. Materials Horizons 2.4 (2015): 420-426.

CPP 26: 2D Materials (Symposium and Joint Session with HL and O): Session II (joint session DS/CPP/HL)

Time: Tuesday 9:30–13:15 Location: H 2032

CPP 26.1 Tue 9:30 H 2032

Structural and electronic interactions in vdW heterostructure MoSe2/few-layer-graphene — •minh tuan dau[1], maxime gay[1], daniela di felice[2], céline vergnaud[1], alain marty[1], cyrille beigné[1], gilles renaud[1], olivier renault[1], pierre mallet[3], toai le-quang[3], jean-yves veuillen[3], loïc huder[1], vincent renard[1], claude chapelier[1], giovanni zamborlini[4], matteo jugovac[4], vitaliy feyer[4], yannick dapp[2], pascal pochet[1], and matthieu jamet[1] — [1]INAC-SPINTEC-PHELIQS-MEM, LETI, CEA/CNRS, Univ. Grenoble Alpes, F-38000 Grenoble, France — [2]SPEC, CEA, CNRS, Univ. Paris Saclay, CEA Saclay, 91191 Gif-sur-Yvette cedex, France — [3]Institut Néel, CNRS, Univ. Grenoble Alpes, F-38000 Grenoble, France — [4]Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich GmbH, D-52425, Jülich, Germany

We have employed surface-sensitive techniques ranging from atomic resolution (STM-STS) to microscopic scale (synchrotron diffraction, photoemission electron microscopy k-PEEM) in order to probe structural and electronic properties of the van der Waals (vdW) heterojuction: MoSe2/few-layer-graphene grown by molecular beam epitaxy. We find that the crystallographic directions of the MoSe2 lattice align perfectly along the ones of graphene, resulting in only one commensurate configuration. Furthermore, we observe a clear evolution of the band structure of the heterojunction compared to the one of bare few-layer-graphene. Indeed, we evidence a large bandgap opening in few-layer-graphene resulting from significant charge transfer between vdW layers.

CPP 26.2 Tue 9:45 H 2032

Interplay of magnetization between graphene and magnetoelectric multiferroics — •Zeila Zanolli — RWTH Aachen Uiniversity, Aachen, Germany

Graphene and magnetoelectric multiferroics are promising materials for spintronic devices with high performance and low energy consumption. We combine the features of both materials by investigating from first principles the interface between graphene and $BaMnO_3$, a magnetoelectric multiferroic. We show [1] that the hybrid systems behaves as a spin filter. Electron charge is transferred across the interface and magnetization is induced in the graphene sheet due to the strong interaction between C and Mn. A remarkably large proximity induced spin splitting of the Dirac cones (300 meV) is achieved and doping can make the high-mobility region of the electronic bands experimentally accessible.

Going further, we investigate spin dynamics at finite temperature using a Monte Carlo approach with exchange coupling parameters fitted from first principles. We find that graphene strongly affects the magnetic properties of the substrate, beyond the interface layer, and induces a softening of the Mn magnetization.

Spin Orbit Coupling calculations reveal that the influence of graphene on the substrate is even more radical and is able to change the direction of the easy axis with respect to the bare $BaMnO_3$ surface. We predict a Rashba splitting of the electronic bands near the K point, and the presence of a Quantum Anomalous Hall effect.

[1] Z. Zanolli, Sci. Rep., 6 (2016) 31346

CPP 26.3 Tue 10:00 H 2032

Gate-Dependent Vacancy Migration in Graphene — •Rohit Babar[1] and Mukul Kabir[1,2] — [1]Department of Physics, Indian Institute of Science Education and Research, Pune, India — [2]Center for Energy Science, Indian Institute of Science Education and Research, Pune, India

Graphene based ultrathin devices offer significant advantage due to their high carrier mobility and a gate-tunable carrier density. However, the experimental observations of vacancy diffusion near room-temperature can potentially lead to undesirable void formation and/or edge modification of such devices. Combining transition state theory with first-principles method, we investigate the microscopic vacancy migration mechanism in graphene and its dependence on gate voltage. The intrinsic vacancy diffusion involves a concerted motion of atoms along with an out-of-plane displacement, which is unique to graphene compared with other 2D materials. We further investigate the migration mechanism under gate voltage and find that the activation barrier non-monotonically increases for both electron and hole doping. The trend in activation barrier is explained via collective-phonon stiffening. We estimate a 10^7-fold decrease in vacancy diffusivity at room temperature. Thus, our findings reveal that the graphene-based devices will not degrade further under device operating condition through vacancy migration.

CPP 26.4 Tue 10:15 H 2032

Transition between rhombohedral and Bernal stacking in multilayer graphene flakes — •Fabian Rudolf Geisenhof[1], Felix Winterer[1], and Ralf Thomas Weitz[1,2] — [1]Physics of Nanosystems, Physics Department, Ludwig Maximilians Universität München — [2]NanoSystems Initiative Munich (NIM) and Center for NanoScience (CeNS)

Quantum transport in multilayer graphene is interesting in many aspects. For example, it was shown that in ultraclean samples of graphene bilayers [1] and recently also multilayers [2], the exchange interaction leads to a novel phase, who's nature is currently still under debate. At the heart of answering this question is knowledge of the local stacking order during charge transport experiments. Here, we show that the fabrication process has an impact on the structural properties of the flakes. It can lead to the formation of ripples and even to a non-local transition from ABC to ABA stacking. This transformation has been identified by spatially resolved Raman and scattering SNOM measurements, and we discuss possible reasons.

[1] R.T. Weitz, M.T. Allen, B.E. Feldman, J. Martin, and A. Yacoby, ”Broken-symmetry states in doubly gated suspended bilayer graphene”, Science 330, 812 (2010)

[2] Y. Nam, D.-K. Ki, M. Koshino, E. McCann and A.F Morpurgo, ”Interaction-induced insulating state in thick multilayer graphene”, 2D Mater. 3 045014 (2016)

CPP 26.5 Tue 10:30 H 2032

Chemical vapour growth and delamination of α-MCl3 nanosheets (M = Ru, Mo, Ti) — •Martin Grönke[1,2], Silke Hampel[1], Peer Schmidt[2], Danny Pohflepp[1], Nadine Bronkalla[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Brandenburg University of Technology Cottbus-Senftenberg, Germany

The two dimensional honeycomb structure of graphene with one monoatomic layer gave an idea to the introduction of other materials with congeneric pattern. Next to carbon based graphene, black phosphorus and binary transition metal chalkogenides, transition metal halides were highly profiled in theory. Among the interest for different materials with strong anisotropic bonding-dependent interactions, resulting frustration effects in honeycomb structures could stabilize new pattern of cooperative magnetic interactions. One candidate to realize a Kitaev Heisenberg (KH) model is the 2D layered honeycomb magnet α-Rutheniumtrichloride (α-RuCl3). Physical properties in nanoscale systems may differ from the respective bulk phase and could even lead to novel physical properties. We herein present to our knowledge the first approach to synthesize phase pure α-RuCl3 crystals on the nanoscale on a substrate via chemical vapour transport (CVT). Beyond that we reveal capabilities to generate thin 2D structures of isostructural compounds like α-MoCl3 and α-TiCl3 on a suitable substrate by means of CVT. Furthermore we show how to increase the number of nanosheets on as grown substrates by different delamination techniques.

CPP 26.6 Tue 10:45 H 2032

Suppression of excitonic absorption in few-layer GaSe — •Arne Budweg[1], Dinesh Yadav[1,2], Alexander Grupp[1], Alfred Leitenstorfer[1], Maxim Trushin[1,3], Fabian Pauly[1,2], and Daniele Brida[1] — [1]Department of Physics and Center for Applied Photonics, University of Konstanz, D-78457 Konstanz, Germany — [2]Okinawa Institute of Science and Technology Graduate University, Onna-son, Okinawa 904-0395, Japan — [3]Centre for Advanced 2D Materials, National University of Singapore, 6 Science Drive 2, Singapore 117546

We study the thickness dependent optical absorption of GaSe via highly sensitive differential transmission measurements. Controlling the number of individual layers in a GaSe nanosheet, we observe a suppression of the excitonic transition below a critical value of 8. Ab-initio modelling enables us to attribute this behavior to a fundamental change in the band structure which, in thin GaSe, leads to a valence band shaped as an inverted Mexican hat. The observed modulation of the optical properties is intrinsic and does not require control via external parameters like substrate material or an applied electric field. Therefore GaSe provides attractive resources for the development of functional optoelectronic devices based on a single material.

CPP 26.7 Tue 11:00 H 2032

Lateral heterostructures for sensing small molecules: electronic current features — Ganesh Sivaraman[1], Frank C. Maier[1], Fabio A.L. de Souza[2], Rodrigo G. Amorim[3], Wanderla L. Scopel[2], Ralph H. Scheicher[4], and •Maria Fyta[1] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Departamento de Fisica, Univer- sidade Federal do Espirito Santo, Brazil — [3]Universidade Federal Fluminense, Departamento de Física, Volta Redonda/RJ, Brazil — [4]Department of Physics and Astronomy, Materials Theory, Uppsala University, SwedenDe

Using density functional theory based calculations with the non-equilibrium Greens functions approach, we study in detail the structural, transport, and electronic properties of two types of lateral 2D heterostructures. The first is a combination of graphene with hexagonal boron-nitride (G/hBN). The second is a (1T) metallic MoS_2 phase embedded in a (2H) semiconducting MoS_2 phase (1T/2HMoS_2). Our results identify the importance of the interface within these materials and provide the relation to the electronic current flowing across these. Having understood the basic properties of these structures, we further reveal their high potential and relevance in detecting small molecules. On one hand, we show that the G/hBN heterostructure can detect small gas molecules. On the other hand, by opening a small pore in the 1T/2HMoS_2 heterostructure, we can distinguish between DNA nucleotides. Proof of both detection schemes is provided through the distinct electronic properties and the clear electronic current signals for the various molecules and each heterostructure.

15 min. break

CPP 26.8 Tue 11:30 H 2032

Thickness dependent electronic and optical properties of TMDCs within many-body perturbation theory — •Philipp Marauhn, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Experimental studies have shown that the spectrum of MoS_2 and other TMDC materials strongly depends on the number of layers of the system. With increasing thickness of a system, the optical absorption spectrum is generally shifted to lower energies.

In this talk we address this behaviour from a theoretical point of view. To investigate the excited electronic states of the TMDCs, we perform three consecutive steps: (i) DFT (ii) *GW* (iii) BSE (Bethe-Salpeter equation). Our results show that both the fundamental quasiparticle gap and the exciton binding energy are significantly reduced when the number of layers is increased. These two effects do not perfectly compensate each other, but lead to an effective shift of the excitation energies towards lower energy. This redshift with increasing number of layers is in agreement with experimental differential reflectance measurements [1]. We also find significant changes in the wave function of some exciton resonances with increasing sample thickness. In multilayer systems, excitons may be composed from electrons and holes situated on different layers, which can be considered as interlayer excitons [2].

[1] Y. Niu et. al., submitted

[2] A. Arora et. al., Nat. Commun., 8(1), 639 (2017)

CPP 26.9 Tue 11:45 H 2032

Elasticity theory for two dimensional systems at finite temperatures — •Johannes Häring and Matthias Fuchs — FB Physik, Universität Konstanz, 78457 Konstanz, Germany

According to the Mermin-Wagner theorem many two dimensional systems only exhibit quasi-long-range order. Recently, we developed an elasticity theory for crystals with point defects and applied it to the defect rich cluster crystal [1]. The theory is able to handle long-range translational order. Now we present a method which includes quasi-long-range order. Furthermore, orientational degrees of freedom are considered as well. As an example results of the helicity modulus and dynamical matrix of the two dimensional XY model are presented. Temperatures range between zero and the Kosterlitz-Thouless transition.

Finally, the influence of topological defects like vortices is discussed.

[1] J.M. Häring, C. Walz, G. Szamel, and M. Fuchs, Phys. Rev. B **92**, 184103 (2015)

CPP 26.10 Tue 12:00 H 2032

Ab Initio Study of the Electronic and Optical Properties of Organic-Inorganic two-dimensional Perovskites: The Role of Many-Body Effects — •Maurizia Palummo[1] and Giacomo Giorgi[2] — [1]INFN and Dip. Fisica University of Roma "Tor Vergata" Via della ricerca scientifica 1 Rome Italy — [2]Dip. Ing. Civile e ambientale Univ. Perugia Italy

Organic-Inorganic Halide Perovskites (OIHPs) represent the most relevant breakthrough in the last decade in photovoltaics (PV) Despite the many attractive features, some serious issues remain that prevent their usage in device mass production, such as the fast air/moisture induced degradatio. For this reason, in the last years two-dimensional Ruddlesden-Popper perovskites (2D-RPOIHPs) have emerged as an alternative to 3D bulk for their superior photo- and chemical-stability coupled with high-performance opto-electronic properties and an enhanced hydrophobic nature of the organic part. While the experimental interest towards this 2D class of materials is nowadays well assessed, ab-initio studies focusing on the role of many-body effects are very limited. By means of a coupled GW plus BSE approach on top of DFT-KS simulations, we here study the electronic and optical properties of a 2D-RPOIHP, as a single sheet and also as a periodic QW. A giant band-gap renormalization of the electronic band-gap and the formation of a strongly bound almost 2D excitons are observed. The relationship between the number of layers is discussed.

CPP 26.11 Tue 12:15 H 2032

Layered van der Waals crystals with hyperbolic light dispersion — •Morten Gjerding — DTU Physics, Fysikvej building 311, 2800 Kgs. Lyngby

Compared to artificially structured hyperbolic metamaterials, whose performance is limited by the finite size of the metallic components, the sparse number of naturally hyperbolic materials recently discovered are promising candidates for the next generation of hyperbolic materials. Using first-principles calculations, we extend the number of known naturally hyperbolic materials to the broad class of layered transition metal dichalcogenides (TMDs). The diverse electronic properties of the transition metal dichalcogenides result in a large variation of the hyperbolic frequency regimes ranging from the near-infrared to the ultraviolet. Combined with the emerging field of van der Waals heterostructuring, we demonstrate how the hyperbolic properties can be further controlled by stacking different two-dimensional crystals opening new perspectives for atomic-scale design of photonic metamaterials. As an application, we identify candidates for Purcell factor control of emission from diamond nitrogen-vacancy centers.

CPP 26.12 Tue 12:30 H 2032

Influence of Hansen solubility parameters on a shear exfoliation process of organophilic layered silica in chloroform — •Michael Huth, Jonas Köhling, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Nanocomposites based on layered silica can be used for several applications, like reinforcement, flame retardant agent, or barrier applications. The understanding of delamination processes of layered silica in organic solvents/polymers is a critical step towards preparing such nanocomposites. In this work, layered silicas with different intercalated molecules are used. Those molecules change the silica surface interaction energies described by Hansen solubility parameters (HSP). HSP of four different synthetic organophilic layered silicas are determined. This allows calculating the dispersibility in chloroform via the Flory-Huggins (F-H) parameter. The F-H parameter can predict the delamination state of organophilic layered silicas in solvents. The delamination state is evaluated quantitatively using atomic force microscopy (AFM). In the case of a high F-H parameter ($\chi > 0.15$), aggregated and unstable layered silica dispersions are found. Whereas in the case of F-H parameters near zero, exfoliated and stable layered silica dispersions are obtained. Additionally, the presence of the surfactant on the surface of fluoromica flakes after exfoliation is proven by Fourier-transform infrared spectroscopy (FT-IR), and density functional theory (DFT) calculations.

CPP 26.13 Tue 12:45 H 2032

Theoretical description of photoemission spectroscopy of van der Waals structures — •Bruno Amorim — CeFEMA, Instituto Superior Técnico, University of Lisbon, Av. Rovisco Pais, PT-1049-001 Lisboa, Portugal

I present a general theory to model the angle resolved photoemission spectroscopy (ARPES) of van der Waals (vdW) structures. VdW structures are formed by lattice mismatched and/or misaligned stacked layers of two-dimensional materials and can be commensurate or incommensurate.

The present theory is based on a tight-binding description of the bound electrons and the concept of generalized umklapp processes, being capable of describing both commensurate and incommensurate structures for arbitrary lattice mismatch/misalignment. In this way, the present theory goes beyond previous descriptions of ARPES in incommensurate vdW structures, which are based on continuous, low energy models, which limits their applicability to structures with small lattice mismatch/misalignment.

As an example, I apply the general method to the case of twisted bilayer graphene, obtaining the ARPES bands and ARPES constant energy maps.

The present theory should be useful in correctly interpreting experimental results of ARPES of vdW structures and other system displaying competition between different periodicities, such as density wave phases.

CPP 26.14 Tue 13:00 H 2032

Manipulating the Mechanical Properties of Ti2C MXene: Effect of Substitutional Doping — •Poulami Chakraborty[1], Tilak Das[2], Dhani Nafday[1], Lilia Boeri[3], and Tanusri Saha-Dasgupta[1] — [1]Department of Condensed Matter Physics and Materials Science, S.N.Bose National Centre for Basic Sciences, JD Block, Sector-3, Salt Lake , Kolkata 700106, India — [2]Department of Physical Sciences, Indian Institute of Science Education and Research-Kolkata, Mohanpur Campus, PO BCKV Campus Main Office, Nadia * 741252, West Bengal, India — [3]Institute for Theoretical and Computational Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria

Two-dimensional transition metal carbides/nitrides $M_{n+1}X_n$ termed as MXenes have attracted immense interest as potential candidates for Li-ion battery anodes and as a hydrogen storage medium. Our work focuses on the specific case of Ti_2C and Ti_2CO_2 under various tensile strain using density functional theory (DFT). We consider substitutional doping of B and V at Ti and C sites of Ti_2C. We have studied substitutional doping with no surface termination as well as oxygen terminated Ti_2C, i.e., Ti_2CO_2. In-plane stiffness, Young's modulus, and critical strain calculations conclude that B doping is highly effective in improving the elastic properties. This trend is found to hold good even for B-doped and V-doped O terminated systems. However the O passivated compounds are found to have relatively higher critical strain values compared to their pristine counterparts. Thus B doped Ti_2CO_2 , $Ti_2(C_{0.5}, B_{0.5})O_2$, appears to be the best candidate among the studied systems, as compared to pure Ti_2C.

CPP 27: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials III (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Tuesday 10:30–13:00 Location: HL 001

CPP 27.1 Tue 10:30 HL 001

Control and prediction of molecular crystal properties by multilevel strategies — •Jan Gerit Brandenburg — London Centre for Nanotechnology, Department of Physics and Astronomy, University College London, 20 Gordon Street, London, U.K.

Computational material science is a dynamic and thriving area of modern scientific research. Approaches based on the fundamental laws of quantum mechanics are now integral to almost any materials design initiative in academia and industry, underpinning efforts such as the Materials Genome initiative or the computational crystal structure prediction [1]. I will present a hierarchy of quantum chemical methods designed for this purpose, in particular targeting molecular crystals and their property prediction. The methods range from high-level diffusion Monte-Carlo (DMC) to London dispersion inclusive DFT, and thus, cover many orders of magnitudes in computational efficiency [2,3]. I will demonstrate the application to the 6th blind test for organic crystal structure prediction. Comparisons to other state-of-the-art methods indicate both success and remaining challenges in the recent method developments [4].

[1] S. L. Price and J. G. Brandenburg, *Molecular Crystal Structure Prediction*; Elsevier Australia, **2017**.

[2] A. Zen, J. G. Brandenburg, J. Klimeš, A. Tkatchenko, D. Alfè, A. Michaelides, **2017**, *submitted.*

[3] J. G. Brandenburg, E. Caldeweyher, S. Grimme, *Phys. Chem. Chem. Phys.* **2016**, *18*, 15519.

[4] A. M. Reilly, et al. *Acta. Cryst. B* **2016**, *72*, 439.

CPP 27.2 Tue 11:00 HL 001

Advances in first-principles and model spin Hamiltonian simulations of point defects in semiconductors for quantum sensors and computing — •Viktor Ivády — Department of Physics, Chemistry and Biology, Linköping University, 581 83 Linköping, Sweden — Wigner Research Center for Physics, Konkoly-Thege Miklós út 29-33, 1121 Budapest, Hungary

First principles simulations play a key role in understanding the physics of point defects in semiconductors, while model spin Hamiltonian approaches are traditionally used to interpret experimental spin dependent observations and describe the spin dynamics of point defects. The development of novel point defect applications, such as quantum bit (qubit) and single photon emitter applications for quantum information processing and quantum sensing, requires detailed understanding of spin-related couplings and addressability of localized defects states in the bath of delocalized electrons that calls for further development and implementation of theoretical tools. Here, I report on my contribution to this field that covers 1) first principles studies for identification of point defect based qubits and single photon emitters , 2) method development for the description of point defects with correlated electron states, 3) implementation of zero-field-splitting calculation for point defect based qubits, 4) development of model spin Hamiltonian approaches for the simulation of optical dynamic nuclear polarization process (ODNP) of point defects, and 5) spin dynamic simulation of existing point defect qubits. As an outlook, I discuss the requirements toward fully-ab initio point defect spin dynamic simulations.

CPP 27.3 Tue 11:30 HL 001

Recent advances in first-principles modelling of correlated magnetic materials — •Yaroslav Kvashnin — Department of physics and astronomy, Uppsala University, BOX 516, 75120 Uppsala

Most of modern first-principles electronic structure studies of correlated materials are based on a combination of density functional theory and dynamical mean field theory (DFT+DMFT).

Addressing magnetic materials within DFT+DMFT has certain peculiarities. There are two recipes one can follow: either to account for magnetism within the DFT functional or to introduce it entirely within the self-energy. Both approaches have their flaws and advantages, which are well-known for DFT+U, but are not often discussed for DFT+DMFT. In my talk I will present a systematic comparison of the two methods and demonstrate the evidences favouring the use of non-polarised functionals.

Next, I will demonstrate how the obtained electronic structure information can be used to simulate finite-temperature magnetic properties in real materials. I employ a so-called two-step approach. First, I map the system on a Heisenberg model and extract the effective exchange parameters Jij's from DFT+DMFT. Then the atomistic spin dynamics simulations are used to simulate magnon spectra and predict the magnetic ordering temperatures.

I will demonstrate the power of such an approach by showing a direct comparison with available experimental data for a wide range of different materials.

CPP 27.4 Tue 12:00 HL 001

A first-principles approach to hot-electron-induced ultrafast dynamics at metal surfaces — •Reinhard J. Maurer — Department of Chemistry, University of Warwick, Gibbet Hill Road, CV4 7AL Coventry, UK

Low-lying electronic excitations in metals, so-called hot electrons, couple efficiently to molecular adsorbate motion. In doing so, they give rise to a number of curious experimental observations. This includes picosecond-scale energy loss of molecular adsorbate vibration, highly inelastic atomic and molecular scattering from metal surfaces, and light-assisted molecular desorption and chemical transformations, recently coined "hot-electron chemistry". In this talk, I will present a first-principles treatment of hot-electron-induced molecular dynamics based on Density Functional Theory that correctly captures the magnitude and mode-specificity of hot-electron mediated adsorbate-substrate energy transfer [1]. Utilizing our efficient all-electron local-orbital implementation of hot-electron-induced frictional forces based on Time-Dependent Perturbation Theory, [2] I will show how we correctly capture vibrational relaxation in large-scale metal-mounted molecular catalysts as well as the energy loss and coupled electron-nuclear dynamics of small molecular adsorbates in both thermal and laser-heated conditions. [3] We scrutinize our approach in comparison to recent Sum-Frequency Generation (SFG) spectroscopy and molecular beam scattering experiments. [1] Phys. Rev. Lett. 116, 217601 (2016) ; [2] Phys. Rev. B 94, 115432 (2017); [3] Phys. Rev. Lett. 118, 256001 (2017);

CPP 27.5 Tue 12:30 HL 001

Temperature effects in spin-orbit physics from first principles — •Bartomeu Monserrat — University of Cambridge, UK — Rutgers University, USA

The spin-orbit interaction drives a number of physical phenomena, including the band inversion in topological insulators and the spin splitting of electronic bands in inversion asymmetric crystals. In this work, we study the effects of finite temperature on such spin-orbit physics, including both thermal expansion and electron-phonon coupling effects [PRB 92, 184301 (2015)].

First, we describe the temperature dependence of the inverted gap in topological insulators. We find that increasing temperature reduces the topological gap in the Bi2Se3 family of materials, and we predict a temperature-induced topological phase transition in Sb2Se3 [PRL 117, 226801 (2016)].

Second, we study the temperature dependence of the spin splitting of electronic bands in both inversion symmetric and asymmetric crystals. We predict a dynamical spin splitting in centrosymmetric crystals and characterise the associated phenomenology in the cubic perovskite CsPbCl3 [arXiv:1711.06274]. In inversion asymmetric crystals, exemplified by the bismuth tellurohalides, we find that increasing temperature suppresses the static spin splitting arising from the Rashba effect [PRM 1, 054201 (2017)].

CPP 28: Condensed Matter Simulations augmented by Advanced Statistical Methodologies I (joint session DY/CPP)

Time: Tuesday 11:00–12:30 Location: BH-N 334

CPP 28.1 Tue 11:00 BH-N 334

Markov State Modeling of Sliding Friction — •Martina Teruzzi — SISSA (International School for Advanced Studies), Trieste

Friction, despite being a well-known and studied phenomenon, still lacks a general theory or approach, mainly due to the presence of many degrees of freedom and the difficulty in identifying few relevant collective variables. We propose a method based on Markov State Modeling, a technique aimed at reducing the dimensionality of the system, by singling out the relevant slow timescales and the observables that best describe them. After successful application to a small toy model (1D Frenkel-Kontorova) we now apply this approach to more complicated systems, identifying few significant states that best characterize them through a rather general and automatic algorithm. This approach can provide insight into the main mechanisms of new frictional systems and, in perspective, could be enhanced by biased sampling to achieve a proper description of rare events, difficult to be sampled by standard dynamics.

CPP 28.2 Tue 11:15 BH-N 334

Loss of Memory in Dense Sheared Particulate Systems — •Lou Kondic[1], Lenka Kovalcinova[1], Miro Kramar[2], and Konstantin Mischaikow[3] — [1]NJIT, Newark, NJ, USA — [2]INRIA Saclay, Paris, France — [3]Rutgers, Piscataway, NJ, USA

We carry out discrete element/MD simulations of dense sheared particulate systems, with the focus on understanding and characterizing dynamical properties of force networks that develop on the mesoscale. These force networks are known to play a crucial role in connecting microscale dynamics of the particles and macroscopic properties of the whole system. The results of the simulations are analysed using topological tools, that allow to fully quantify and even compare the states of the system. These tools identify in an objective and precise manner the time interval needed for the system to loose its memory, or in other words, the time interval after which any information about system state is lost. We will show that the process of memory loss may differ even if the inertial number, measuring the ratio of inertial to imposed forces, is kept constant.

This work is supported by the NSF Grant No. DMS-151717 by the DARPA contract No. HR0011- 16-2-0033.

CPP 28.3 Tue 11:30 BH-N 334

Adaptive population Monte Carlo simulations — •Martin Weigel[1], Lev Yu. Barash[2,3], Lev N. Shchur[2,3,4], and Wolfhard Janke[5] — [1]Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, England — [2]Landau Institute for Theoretical Physics, 142432 Chernogolovka, Russia — [3]Science Center in Chenogolovka,142432 Chernogolovka, Russia — [4]National Research University Higher School of Economics, 101000 Moscow, Russia — [5]Institut für Theoretische Physik, Universität Leipzig, Postfach 100920 04009, Leipzig, Germany

Population annealing is a sequential Monte Carlo scheme that is potentially able to make use of highly parallel computational resources. Additionally, it promises to allow for the accelerated simulation of systems with complex free-energy landscapes, much alike to the much more well known replica-exchange or parallel tempering approach. We equip this method with self-adaptive schemes for choosing the algorithmic parameters, including the temperature and sweep protocols as well as the population size. The resulting method is significantly more efficient for simulations of systems with complex free-energy landscapes than some more traditional approaches, and it is particularly well suited for massively parallel computing environments such as (clusters of) GPUs.

CPP 28.4 Tue 11:45 BH-N 334

Diagnostics of neural networks for machine learning phases and phase transitions — •Philippe L. Suchsland and Stefan Wessel — RWTH Aachen University, Aachen, Germany

Machine learning schemes based on neural networks have recently been proposed as new tools for classifying phases of matter as well as detecting phase transitions. One motivation behind such proposals is the ability of appropriately designed and trained neural networks to identify patterns from a large set of data without having to explicitly describe them. We apply both supervised and unsupervised machine learning schemes to basic models of statistical physics. In particular, we consider the 2D Ising model in the presence of extended domain-wall configurations as well as the 2D XY model that exhibits a Kosterlitz-Thouless transition. In both cases, we identify the physical properties of the models that are relevant for the classification task. This reveals how reliable these schemes are with respect to minimizing the amount of preprocessing of bare sample configurations before feeding them into the learning process.

CPP 28.5 Tue 12:00 BH-N 334

Hyperdynamics approach to the non-equilibrium states coupled to the thermal bath — •Yuri S. Nagornov and Ryosuke Akashi — University of Tokyo, Department of Physics, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

Efficient numerical simulation method for rare events driven by thermal fluctuation has long been a hot topic in a wide range of fields in condensed-matter physics. The target phenomena in this context, such as crystal nucleation, atomic diffusion etc., occur in time scales of microseconds or even longer and are intractable by atomistic molecular dynamics simulation. Solutions to this problem have long been attempted by introducing collective variables to seek for escape paths and/or efficiently sampling the phase space to represent the canonical ensemble. However, an ideal approach is rather desired (i) not to respect the prior knowledge of appropriate collective variables and (ii) not to require the system to reach the thermal equilibrium since many of the above mentioned phenomena can occur under non-equilibrium situations. Along the line of the Langer*s theory, we formulate a differential equation for the distribution of the variables that evolve on an elevated potential surface under thermal fluctuation, from which its real probability of realization can be retrieved. This formalism enables us non-empirical exploration of rare events and evaluation of its probability to occur simultaneously. An algorithm with a modified form of the Langevin molecular dynamics is thereby constructed, which is in spirit an extension of the hyperdynamics approach. Applications to simple model systems will be presented.

CPP 28.6 Tue 12:15 BH-N 334

Hyperdynamics approach to the non-equilibrium states coupled to the thermal bath — •Yuri S. Nagornov and Ryosuke Akashi — University of Tokyo, Department of Physics, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

Efficient numerical simulation method for rare events driven by thermal fluctuation has long been a hot topic in a wide range of fields in condensed-matter physics. The target phenomena in this context, such as crystal nucleation, atomic diffusion etc., occur in time scales of microseconds or even longer and are intractable by atomistic molecular dynamics simulation. Solutions to this problem have long been attempted by introducing collective variables to seek for escape paths and/or efficiently sampling the phase space to represent the canonical ensemble. However, an ideal approach is rather desired (i) not to respect the prior knowledge of appropriate collective variables and (ii) not to require the system to reach the thermal equilibrium since many of the above mentioned phenomena can occur under non-equilibrium situations. Along the line of the Langer's theory, we formulate a differential equation for the distribution of the variables that evolve on an elevated potential surface under thermal fluctuation, from which its real probability of realization can be retrieved. This formalism enables us non-empirical exploration of rare events and evaluation of its probability to occur simultaneously. An algorithm with a modified form of the Langevin molecular dynamics is thereby constructed, which is in spirit an extension of the hyperdynamics approach. Applications to simple model systems will be presented.

CPP 29: Nanostructures, Nanostructuring and Nanosized Soft Matter I

Time: Tuesday 11:15–13:00 Location: C 230

CPP 29.1 Tue 11:15 C 230

Strain-induced formation of oriented plasmonic oligomers on elastomeric substrate — •Anja Maria Steiner[1,2], Martin mayer[1,2], Maximilian Seuss[1], Svetoslav Nikolov[3], Alexander Alexeev[3], Christian Kuttner[1,2], Tobias A.F. König[1,2], and Andreas Fery[1,2,4] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [2]Centre for Advancing Electronics Dresden, Germany — [3]Georgia Tech, Atlanta, United States — [4]Department of Physical Chemistry of Polymeric Materials, TU Dresden, Germany

We present the formation of oriented chains of few plasmonic nanoparticles,so called plasmonic oligomers, by controlled fragmentation of linear particle assemblies into finite sub-chains. Detailed investigations of the fragmentation process are conducted by in-situ atomic force microscopy (AFM) and correlated to UV-vis-NIR spectroscopy. By evaluation of the strain dependent optical properties we found a reversible, non-linear shift of the dominant plasmonic resonance. Based on the AFM measurements, the optical evaluation and mechanical modeling (lattice spring method), we prove a formation mechanism which provides experimental guiding lines. Following this strain-dependent fragmentation mechanism the chain length can be controlled depending on the ratio of cohesion between the particles and adhesion of the colloids to the supporting elastomeric substrate. We demonstrate, that mechanical stimulus is a powerful tool for the scalable fabrication of oriented linear plasmonic oligomers and opens new avenues for strain-dependent optical devises and mechanoplasmonic applications.
A.M. Steiner *et al.*,ACS Nano, **2017**, 11, 8871–8880

CPP 29.2 Tue 11:30 C 230

Plasmonic Broadband Absorbers for Hot Electrons Extraction — •Charlene Ng[1], Ann Roberts[2], Tim Davis[2], Daniel Gomez[3], Tobias König[1], and Andreas Fery[1] — [1]Leibniz-Institut für Polymerforschung, Institiute of Physical Chemistry and Polymer Physics, Dresden, Germany — [2]School of Physics, The University of Melbourne, Victoria, Australia 3010 — [3]RMIT University, Melbourne, VIC, 3000, Australia

Metallic nanostructures exhibit localized surface plasmon resonances (LSPR), a phenomenon where the confined electrons of the metal collectively oscillate in response to the interaction with light. Following the excitation of LSPRs, the energy flow out radiatively though reemitted photons or non-radiatively by generating highly energetic hot electrons. When in contact with a semiconductor, plasmonic nanostructures can form a Schottky junction and could emit these hot electrons to the conduction band of semiconductor, where various photo-induced chemical reactions can be induced. Most importantly, the generation of these hot electrons usually requires photon energies that are much lower than the band gap energy of typical semiconductors, allowing visible or near infra-red light to be harnessed. This emerging approach for harvesting solar energy essentially opens up new strategies to achieve high performance photocatalytic devices. Essentially, the first step to achieve high conversion efficiencies is to maximise the light absorption of plasmonic metal nanostructures. In this work, different strategies to maximise the light absorption of plasmonic nanostructures and efficient extraction of hot electrons will be discussed.

CPP 29.3 Tue 11:45 C 230

Systematic investigation of the coherent light coupling in various nanocavity geometries — •Fabian R. Gossler[1,2], Max J. Schnepf[1], and Tobias A.F. König[1,2] — [1]Institute of Physical Chemistry and Polymer Physics, Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden — [2]Cluster of Excellence Centre for Advancing Electronics Dresden, TU Dresden, Germany

We are interested in the interaction of light with self-assembled plasmonic cavities. In such film coupled nanoparticle structures, we will couple quantum emitters with plasmonic systems of various geometries such as spheres, cubes and anisotropic particles to study the coherent energy transfer. The self-assembly of metallic nanoparticles on a plasmonic film features a high optical quality in comparison to top-down lithography fabrication methods. Moreover, we tune the radiative process by modifying the cavity size through a polyelectrolyte multilayers approach with embedded Rhodamin B fluorophores. We employ atomic force microscopy, dark field scattering spectroscopy, fluorescence life-time imaging and TCSPC at the same cavity to show decreases in the fluorescence life-time as well as emission intensity enhancement of several orders of magnitude. Finally, we support the results with FDTD simulations for quantitative evaluation of the occurring plasmonic modes as well as the radiative and non-radiative decay rates. As an outlook, we present a robust self-assembly method supported by laser interference lithography templates to fabricate a plasmonic lattice for coherent energy transfer on macroscopic scales.

CPP 29.4 Tue 12:00 C 230

Coherent energy transfer in a plasmonic colloidal nanocavity

— •Max J. Schnepf[1,2], Yannic Brasse[1,2], Fabian R. Gossler[1,2], Andreas Fery[1,2,3], and Tobias A.F. König[1,2] — [1]Leibniz Institute of Polymer Research (IPF), Institute of Physical Chemistry and Polymer Physics, Hohe Str. 6, 01069 Dresden, Germany — [2]Cluster of Excellence Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, Germany — [3]Physical Chemistry of Polymeric Materials, Technische Universität Dresden, Germany

We present a film-coupled colloidal building-block, comprising of a plasmonic core surrounded by a dielectric shell containing a fluorophore emitter. Due to the small mode volume and the strong loss rate, the system is considered to be in a strong coupling regime. As a result, fluorescent lifetime of the emitter is significantly reduced and the emission rate is enhanced while the energy of the emitted photons remains unaffected.

We systematically study the energy transfer mechanism on the single particle level by employing electron microscopy, scattering spectroscopy, fluorescence life-time imaging (FLIM) and time-correlated single photon counting on the same cavity. Supported by finite-difference time-domain simulations, we examine the efficiency and nature of the energy transfer effects. Finally, we discuss the future direction in coupling of these building blocks into a plasmonic lattice.

CPP 29.5 Tue 12:15 C 230

Nanostructure and optical properties of spray-deposited metal-organic decomposition inks — •Stephan V. Roth[1,2], Björn Fricke[1], Calvin Brett[1,2], Wiebke Ohm[1], Andre Rothkirch[1], Matthias Schwartzkopf[1], and Tim Laarmann[1,3] — [1]DESY, Notkestr. 85, 22607 Hamburg — [2]KTH Royal Institute of Technology, 10044 Stockholm, Sweden — [3]CUI, Luruper Chaussee 149, 22761 Hamburg 22761, Germany

Metal-organic decomposition inks offer a facile route for preparing functional nanoparticle and conductive coatings based on precursor and solvent-based methods. Using spray deposition as roll-to-roll compatible coating method [1], we investigated the spray deposition of the silver nitrate precursor and the subsequent transformation into metallic silver layers via thermal annealing in situ and in real-time. We employed a combination of surface sensitive time-resolved wide- and small-angle x-ray scattering and optical spectroscopy. Thus, we followed the nanostructuring and the transformation of the deposited precursor into deposited metallic silver nanoparticles and correlate the occurring plasmon resonance to the nanoparticulate layer morphology. This is indispensable for optimizing the coating by tuning the deposition and annealing parameters for future use as sensors [2]. [1] S. V. Roth, J. Phys.: Condens. Matter 28, 403003 (2016) [2] G. Santoro et al., Appl. Phys. Lett 104, 243107 (2014)

CPP 29.6 Tue 12:30 C 230

From Single Particles to Coupled Plasmonic Systems — •Martin Mayer[1,2], Pavel Potapov[3], Anja Maria Steiner[1,2], Axel Lubk[3], Tobias A.F. König[1,2], and Andreas Fery[1,2,4] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [2]Center for Advancing Electronics Dresden, Germany — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany — [4]Department of Physical Chemistry of Polymeric Materials, TU Dresden, Germany

Despite being often considered as analogous plasmonic antennas, the behavior upon elongation as well as the nature of the near-field plasmonics of nanowires and coupled particle chains differ drastically. While nanowires shift linearly with elongation and build up standing surface charge waves, particle chains (plasmonic polymers) converge to a specific energy (infinite chain limit) at relatively few particles and the resulting near-field plasmonics is dominated by the formation of an energy band.

By exploiting wet-chemical synthesis under living reaction conditions and template-assisted colloidal self-assembly, respectively, we compare the far-field (UV-vis-NIR) and near-field (EELS) behavior of these systems with the support of electromagnetic simulations.
M. Mayer *et al., Nano Lett.*, **2015**, 15, 5427–5437.
M. Mayer *et al., Angew. Chem.,* **2017**, DOI: 10.1002/anie.201708398.
A.M. Steiner *et al., ACS Nano,* **2017**, 11, 8871–8880.

CPP 29.7 Tue 12:45 C 230

Spray-mediated shear forces versus topographical confinement: controlling the orientation of silver nanowires — •Patrick T. Probst[1], Sribharani Sekar[1,2], Tobias A.F. König[1,3], Petr Formanek[1], Gero Decher[2], Andreas Fery[1,3], and Matthias Pauly[2] — [1]Leibniz-Inst. für Polymerforschung Dresden e.V., Germany — [2]Université de Strasbourg, CNRS, Inst. Charles Sadron, France — [3]Centre for Adv. Electronics Dresden, Germany

Grazing Incidence Spraying is known to enable linear arrangement of 1-dimensional nanoparticles facilitated by the arising shear forces. That way, optically and electrically anisotropic thin films of a vast variety of materials (metal, semiconductor, nanofibrils) can be readily produced on macroscopic scales (>5×5 mm^2).

Surprisingly, parallel surface corrugations on the receiver substrate not only render the process more robust against rotational offsets during preparation, but, more interestingly, they can even reorient the particles by 90° to be parallel to the corrugations again. Controlling the balance between shear forces and topographical confinement opens new ways for constructing complex nano-patterns. We show how the microscopic linear arrangement of AgNWs evaluated by scanning electron microscopy (order parameter >0.9) reflects in a pronounced macroscopic optical anisotropy measured by conventional polarized UV-Vis-NIR spectroscopy.

S. Sekar, V. Lemaire, H. Hu *et al. Faraday Discuss.* **2016,** *191,* 373.
H. Hu, M Pauly, O. Felix *et al. Nanoscale* **2017,** *9,* 1307.
S. Sekar, P.T. Probst, M. Pauly *et al., submitted.*

CPP 30: Friction and Rheology

Time: Tuesday 11:45–13:00 Location: C 264

Invited Talk CPP 30.1 Tue 11:45 C 264

Novel hyphenated rheology techniques for the study of quiescent and flow-induced polymer crystallization — Volker Räntzsch, Mürüvvet Begüm Özen, Karl-Friedrich Ratzsch, Gisela Guthausen, and •Manfred Wilhelm — Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Combining rheology with *in-situ* characterization techniques has received great attention in the past 30 years because such combinations lead to correlated information on flow properties, molecular dynamics and microstructure of soft matter such as polymers, liquid crystals or colloids. Additionally, flow profiles both in the linear and non-linear regime can be applied to monitor and also to modify the state of a sample and measure its implications on molecular dynamics and microstructure. Here we present novel hyphenated set-ups including RheoNMR and RheoSAXS. These unique combinations can be employed to simultaneously conduct a full rheological characterization (G', G'', $|\eta^*|$, etc.) while monitoring molecular dynamics via ^{1}H TD-NMR and nanoscale structure via 2D-SAXS for temperatures up to +210 °C. Possible applications for hyphenated rheology techniques include the measurement of crystallizing soft matter (fats, polymers, etc.) and multiphase systems during the application of shear protocols. To display the possibilities of these new techniques, studies on the quiescent and flow-induced crystallization of polyolefins are presented.

CPP 30.2 Tue 12:15 C 264

Measuring lateral force on soft and stiff materials with Intermodulation AFM — •Per-Anders Thorén, Riccardo Borgani, Daniel Forchheimer, and David B. Haviland — Department of Applied Physics, KTH Royal Institute of Technology Stockholm SE-106 91, Sweden

We present a technique [1] for measuring the velocity-dependence of frictional forces on a single asperity (an AFM tip) reaching velocities up to several cm/s. The method is based on the measurement and analysis of intermodulation products, or frequency mixing of multiple drive tones near a high Q torsional resonance, which arise from the nonlinear frictional force. The method gives the oscillation amplitude dependence of both conservative and dissipative dynamic force quadratures, revealing the transition between static and dynamic friction at the nanometer scale. We show measurements on a stiff mica sample and for a few different soft polymer surfaces such as PDMS and a PS-LDPE-blend. Using a modified Prantl-Tomlinson model [1], we simulate the interaction of the cantilever and its tip with the mica-surface. The softer polymer surfaces are discussed in terms of a moving surface model [2], where the finite relaxation time of the lateral deformation of the viscoelastic surface gives rise to the hysteresis seen in the force quadrature curves.

[1]: P-A. Thorén et al., Nat. Commun. 7, doi:10.1038/ncomms13836 (2016)

[2]: P-A. Thorén et al., arXiv http://arxiv.org/abs/1711.09024 (2017)

CPP 30.3 Tue 12:30 C 264

The transition from hydrodynamic via interfacial to dry friction for sheared surfaces in water — •Alexander Schlaich[1,2], Julian Kappler[1], and Roland R. Netz[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Laboratoire Interdisciplinaire de Physique (LIPhy), CNRS and Université Grenoble Alpes, F-38000 Grenoble, France

The friction force between hydrated surfaces under shear is important in various fields ranging from biolubrication to flocculation and jamming. For large surface separation friction is well described by hydrodynamics and dominated by the water viscosity. As the normal pressure increases the surface separation goes down, leading to water properties that differ drastically from bulk and where the interfacial viscous properties dominate, thus modifying the friction force. When the normal pressure is so high that all water is squeezed out, dry friction is obtained.

We establish the general framework that describes the separation-dependent crossover between these three regimes. We concentrate on neutral yet polar membrane-like surfaces which exhibit stable water films and are governed by strong hydration repulsion and report extensive atomistic non-equilibrium molecular dynamics simulations. In that case it is important to correctly account for the constant water chemical potential as the water number changes according to the applied normal pressure.

CPP 30.4 Tue 12:45 C 264

Microliter viscometry using a bright-field microscope: η-DDM — Manuel A. Escobedo-Sanchez[1], Juan-Pablo Segovia-Gutierrez[1], Angel B. Zuccolotto-Bernez[2], Jan Hansen[1], Caroline-C. Marciniak[1], Katrin Sachowsky[1], •Florian Platten[1], and Stefan U. Egelhaaf[1] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Departamento de Física, CINVESTAV-IPN, México D.F, Mexico

Passive microrheology can be considered as the counterpart of bulk small amplitude oscillatory shear measurements at the microscale. Microrheology exploits the Brownian motion of colloidal tracer particles. The mean-squared displacement (MSD) of the tracers is related to the rheological and viscometric properties of the suspension. It is commonly determined by particle tracking, which requires a careful selection of tracer trajectories. In contrast, Differential Dynamic Microscopy (DDM) avoids particle tracking and hence its limitations while still allowing for microliter-sized samples. DDM exploits the spatial Fourier transform of image differences which provides access to the MSD via the intermediate scattering function that is commonly acquired in dynamic light scattering experiments. We propose to combine DDM with the empirical Cox-Merz rule to estimate the steady shear viscosity of biological and soft matter systems. This technique even is applicable when reliable steady shear measurements are hard to achieve due to the torque resolution limit. Hence, an optical microscope can be used as a convenient and reliable microliter viscometer.

CPP 31: Modeling and Simulation of Soft Matter I (joint session CPP/DY)

Time: Tuesday 14:00–16:00 Location: PC 203

Invited Talk CPP 31.1 Tue 14:00 PC 203

The role of correlations in the collective behaviour of microswimmer suspensions — •Alexander Morozov — University of Edinburgh, Edinburgh, UK

Recent years witnessed a significant interest in physical, biological and engineering properties of self-propelled particles, such as bacteria or synthetic microswimmers. The main distinction of this 'active matter' from its passive counterpart is the ability to extract energy from the environment (consume food) and convert it into directed motion. One of the most striking consequences of this distinction is the appearance of collective motion in self-propelled particles suspended in a fluid observed in recent experiments and simulations: at low densities particles move around in an uncorrelated fashion, while at higher densities they organise into jets and vortices comprising many individual swimmers. Although this problem recieved significant attention in recent years, the precise origin of the transition is poorly understood.

In this talk I will present a numerical method based on a Lattice-Boltzmann algorithm to simulate hydrodynamic interactions between a large number of model swimmers (order 10^5), represented by extended force dipoles. Using this method we simulate dilute suspensions of self-propelled particles and show that, even below the transition, swimmers move in a correlated fashion that cannot be described by a mean-field approach. We develop a novel kinetic theory that captures these correlations and is non-perturbative in the swimmer density, and reveals the asymmetry between pusher and puller swimmers below the transition to turbulence.

CPP 31.2 Tue 14:30 PC 203

Polymer Topology by Chain Walking Polymerization Catalysis — •Ron Dockhorn[1,2], Albena Lederer[1], Jan Merna[3], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany — [3]University of Chemistry and Technology Prague, CZ-16628 Praha, Czech Republic

Monte Carlo simulations of the chain walking polymerization catalysis (CW) are performed using the bond fluctuation model to investigate the influence of the walking mechanism on the polymer topology at a given molecular weight. In agreement to previous findings, for high reaction probability/slow walking the structure growths with linear chain extensions. On the other hand, for low reaction probability/fast walking the structures show dendritic growth of the polymer. The transition region is characterized by large amount of branched side chains reflecting a cross-over regime with linear global features and dendritic local sub-structures. This is in contrast to the Zimm-Stockmayer hyperbranched (ZS-HB) scaling. Static properties are investigated by means of radius of gyration and scattering function of perfect dendrimers, ZS-HB, and CW-structures. A generalized mean-field model is applied, and is found in fair agreement with the simulation data under good solvent conditions. These findings are aimed to understand the physical properties related with the topology of the CW-structures to improve the synthesis of a new class of hyperbranched molecules.

CPP 31.3 Tue 14:45 PC 203

Understanding the Dynamical Behavior of Twin Polymerization — Constantin Huster, Halit Taskin, and •Janett Prehl — Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany

Twin polymerization enables the formation of two different macromolecular structures of organic-inorganic hybrid materials in one single process step. To investigate the dynamical behavior and the morphology of the reaction process and the final compounds we recently developed a Monte-Carlo based reactive bond fluctuation model (rBFM) [1] that is capable to cope with the complexity of the underlying reaction mechanism. Special feature of this rBFM is the possibility to define multiple reaction centers per monomer and multiple bond vectors between two monomers that exhibit different properties.

In this presentation we introduce the rBFM and analyze first results of the diffusive behavior of the reacting twin monomers over time. By doing so we gain insights into the structure formation process of twin polymerization.

[1] K.H.Hoffmann, J.Prehl, *Reac Kinet Mech Cat* DOI: 10.1007/s11144-017-1303-y

CPP 31.4 Tue 15:00 PC 203

Bridging Time Scales with Variationally Enhanced Sampling — •Omar Valsson — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany

The usefulness of atomistic simulations is generally hampered by the presence of several metastable states separated by high barriers leading to kinetic bottlenecks. Transitions between metastable states thus occur on much longer time scales than one can simulate. Numerous enhanced sampling methods have been introduced to alleviate this time scale problem, including methods based on identifying a few crucial order parameters and enhancing their sampling through the introduction of an external biasing potential.

Here will we discuss Variationally Enhanced Sampling (Valsson and Parrinello, PRL 113 090601, 2014), a generally applicable enhanced sampling method where an external bias potential is constructed by minimizing a convex functional. We present numerous examples from physics and chemistry which show the flexibility and practicality of the method. We will furthermore show how the variational property of the method can be used to extend the method in various innovative ways, e.g.: to obtain kinetic information from atomistic simulation; to accelerate nucleation events by employing models from classial nucleation theory; and to incorporate experimental information into molecular simulations.

We will also introduce the VES code (http://www.ves-code.org), an open-source library for the PLUMED 2 plugin that implements methods based on Variationally Enhanced Sampling.

CPP 31.5 Tue 15:15 PC 203

Kinetics of defects in self-assembled block-copolymers using continuum models — •Juan Carlos Orozco Rey and Marcus Mueller — University of Goettingen, Institute of Theoretical Physics, Goettingen, Germany

The computational study of directed self-assembled (DSA) of copolymeric materials is a challenging task due to the disparity of length scales involved in the structure formation process. Fast simulation techniques, which enable us to conciliate the periodicity of the self-assembled structures with the large scale of devices targeted in the manufacturing of these materials, are of significant interest. Continuum models provide the highest level of coarse-graining where the polymer system is no longer described by the molecular degrees of freedom but only in terms of a local collective variable - the difference in composition. We study the ability of two continuum models - Ohta-Kawasaki and Swift-Hohenberg - to describe key aspects of defects and their dynamics: the limits of stability, the shape of the internal AB interfaces and the kinetics of motion.

We use particle-based simulations and self-consistent field theory to compare and identify the most promising model for the study of DSA. We show that in spite of the caveats of a highly coarse-grained description, a continuum model provides valuable insights into the kinetics of self-assembly as well as into the surface-directed structure formation of device-oriented structures like T-junctions. The combination with more detailed models enables us to gain better understanding of the process while reducing the computational cost.

CPP 31.6 Tue 15:30 PC 203

Higher coordination of cross-links improve toughness of fiber bundles — •Huzaifa Shabbir and Markus Hartmann — Sensengasse 8 , 1090 Vienna Austria

(Physical) cross-linking is an effective strategy to tailor the mechanical properties of polymeric systems. Often, these cross-links are weaker than the covalent backbone that holds the structure together. If reversible, cross-links provide the material with some self-healing behavior.

We use Monte Carlo simulations to investigate the mechanical behavior of (reversibly) cross-linked polymeric systems. The framework of a multi-body potential is utilized to control the coordination of cross-links (coordination is defined as the number of monomers participating in one cross-link). Displacement controlled computational loading experiments are conducted to evaluate the mechanical properties of fibrous systems.

Previous work shows that the coordination of cross-links significantly influences the mechanical performance of a linear chain [1]. In this talk, the influence of the coordination of cross-links on the mechanics of aligned fiber bundles will be discussed. In particular, it will be shown that the coordination of cross-links has a large impact on the toughness of fiber bundles as higher coordination inhibits the premature rupture of the covalent backbone observed for classical cross-links of two fold coordination [2]. Special emphasis will be put on the influence of the topology of cross-links that show a much richer variety for a higher coordination compared to the classical coordination of two.

CPP 31.7 Tue 15:45 PC 203

Permeability maximization in polymer gels: Modeling and simulation — •Won Kyu Kim[1], Matej Kanduč[1], Rafael Roa[1], and Joachim Dzubiella[1,2] — [1]Institut für Weiche Materie und Funktionale Materialien, Helmholtz-Zentrum Berlin, Berlin, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany

Permeability measures the ability of soft matter, such as polymer-based networks (hydrogels), to transport solvents and solutes, defining important control parameters in soft functional material applications, e.g., for filtration, drug release, and transport of reactants in responsive nano-reactors [1-4]. We study permeability by means of coarse-grained simulations and theory of a model polymer network. We find that the permeability can be maximized by optimal polymer volume fractions and inter-particle interactions between the polymer and the penetrating solutes. This nontrivial phenomenon is triggered by a competition between solute partitioning [1-3] and diffusion [2]. Throughout a wide range of parameter space of the solvent quality, solute coupling, and gel volume fraction, a rich topology of the partitioning is found. The solutes' diffusivity is highly correlated to gel structures, resulting in a drastically nonmonotonous permeability. Possible applications to hydrogel based devices such as responsive nanoreactors for catalysis [2,4] are discussed.

[1] W. K. Kim et al, Macromolecules 50, 6227 (2017). [2] R. Roa et al, ACS Catalysis 7, 5604 (2017). [3] M. Kanduč et al, Phys. Chem. Chem. Phys. 19, 5906 (2017). [4] S. Wu et al, Angewandte Chemie 51, 2229 (2012).

CPP 32: Poster Session II

Topics: Smart Hydrogels and Hydrogel-Based Devices (32.1-32.5), Hydrogels and Microgels (32.6-32.13).

Time: Tuesday 14:00–16:00 Location: Poster B

CPP 32.1 Tue 14:00 Poster B

Structural investigations of multi-responsive physical hydrogels — •Florian Jung[1], Panayiota A. Panteli[2], Constantinos Tsitsilianis[3], Costas S. Patrickios[2], and Christine M. Papadakis[1] — [1]Technical University of Munich, Physics Department, Garching, Germany — [2]University of Cyprus, Department of Chemistry, Nicosia, Cyprus — [3]University of Patras, Department of Chemical Engineering, Patras, Greece

Stimuli-responsive physical hydrogels strongly change their properties upon a small change of the environment and may be used as fast sensors or for drug delivery.

In the present work, we investigate the structure of a multiresponsive, CBABC type pentablock terpolymer. The end blocks are statistical copolymers of the hydrophobic n-BuMA and the thermoresponsive TEGMA, the intermediate middle blocks are the weak cationic polyelectrolyte PDMAEMA, and the middle block is the hydrophilic PEG. In aqueous solution, either flower-like micelles or a physical network, with the hydrophobic end blocks acting as crosslinks, are expected. The dynamics of the network may be tuned by varying the temperature around the cloudpoint. pH allows stretching of the intermediate blocks and thus tunes the gelation behavior. Concentration-, pH- and temperature-dependent structural information was obtained from dynamic light scattering (DLS) and small-angle X-ray scattering (SAXS) investigations. The results show that there is an interplay between different responses in these multiresponsive systems.

CPP 32.2 Tue 14:00 Poster B

Poisson-Boltzmann Cell Model for Swelling of Macroscopic Polymer Gels — •Jonas Landsgesell, Patrick Kreissl, and Christian Holm — Institute for Computational Physics Universität Stuttgart Allmandring 3 70569 Stuttgart Germany

Polymer gels can swell tremendously when exposed to aqueous solutions. Recent experiments and theoretical work showed that polymer gels can even be used to desalinate sea water. In this context adequate modeling of the free energy is important for predicting e.g. the energetic costs for desalinating sea water. For an improved energetic description we developed a Poisson-Boltzmann (PB) model for polymer gels. This model allows e.g. the prediction of the the swelling equilibrium of charged polyelectrolyte gels via solving numerically the PB cell model in the presence of salt. We compare the results of the cell model with previous results of Molecular Dynamics simulations.

CPP 32.3 Tue 14:00 Poster B

Sophisticated Techniques to Implement Hydrogel Components into Microsystems — •Anthony Beck, Philipp Jan Mehner, Philipp Frank, Sebastian Häfner, Georgi Paschew, and Andreas Richter — Technische Universität Dresden, Institute of Semiconductors and Microsystems, Chair of Microsystems, 01062 Dresden, Germany

The successful miniaturization and commercialization of fully integrated microfluidic systems with monolithic active-material components is still under development. For example, feasible micro-valve concepts have been demonstrated that show promising potential for high integration on lab-on-chips and other applications. Due to the wide range of synthesis procedures, design parameters and the challenge to develop reproducible hydrogel-based components, the high degree of integration of hydrogels still cannot accomplish the expectations which were made by many researches.

We propose a reliable, systematic investigation on lithographical structuring hydrogels and MEMS-compatible fabrication techniques which make it possible to simultaneously and quickly integrate many different hydrogel-based components in one system. In the field of microfluidics, the channel shapes, number and geometry of various hydrogel-based valves and diodes have been evaluated experimentally to improve performance parameters. The proposed designs extend the application possibilities with back pressures of up to 1 bar. Important design rules for next generation highly integrated microfluidic components are formulated.

CPP 32.4 Tue 14:00 Poster B

Janus emulsions and Janus gels stabilized by polyelectrolyte complexes — •Rajarshi Roy Raju, Sabine Kosmella, and Joachim Koetz — Institut für Chemie, Universität Potsdam, Karl-Liebknecht-Strasse 24-25, D-14476, Potsdam, Germany

Janus emulsion is a special kind of emulsions which contains emulsion droplets composed by two hemispheres of immiscible oils surrounded by water. Our research activities deal with the formation of Janus emulsions through moderate-energy vibrational emulsification of olive oil and silicone oil in presence of polyelectrolytes, polyelectrolyte complexes and metallic nanoparticles stabilizing the individual oil droplets. Therefore, we have investigated the pH dependence of polyelectrolytes, e.g., chitosan, Na-carboxymethylcellulose (NaCMC), gelatin and Na-polyacrylate (NaPAA), and their possibility to form well defined polyelectrolyte complexes. By using chitosan one can find a pH-dependent fine-tuning of the Janus droplet size. By adding gelatine/NaPAA complex particles, varying in the particle size between 200 and 400 nm, it was possible to tune the Janus emulsion droplet diameter between 50 and 200 μm. Cryo-SEM images of the Janus droplets confirm the adsorption of complex particles on olive oil interface leading to a substantial decrease of the interfacial tension. Furthermore, Janus emulsion turns into a long-term stable Janus gel in presence of gelatine/NaCMC composites. In this case, Janus droplets remain embedded in the gel network and show elastic rheological behaviour along with noticeable thixotropic properties.

CPP 32.5 Tue 14:00 Poster B

Modified Network Description Model of a Hydrogel-based Microvalve with Static and Transient Material Behavior for Parameter Variation Studies — •Philipp J. Mehner, Anthony Beck, Dai Zhongke, Andreas Voigt, Uwe Marschner, and Andreas Richter — Chair of Microsystems, Technische Universität Dresden, Germany

A hydrogel-based microvalve is a device which can be used for flow control in microfluidic systems either by an external source like heat or by fluidic stimuli like concentration levels or ph value. These microvalves show a transistor-like behavior and, comparable to the microelectronics field, open the possibility for highly integrated chips. This creates the need for a design environment to model the fluid behavior of microfluidic chips and requires furthermore a description of the behavior of the hydrogel in the valve as well as its interaction with the trigger domain.

We propose an updated network description model which is capable of efficiently computing an arbitrary number of hydrogel-based microvalves. The benefit is, that trigger interactions and swelling rates are included within the model and flow results can be probed for every individual microvalve. Hydrogel material behavior is implemented for the transient as well as the quasistatic swelling regime. Efficient parameter studies are now feasible and demonstrated. With this tool, it is possible to model highly integrated microfluidic circuits, such that design ideas can be tested first and can then be verified experimentally.

CPP 32.6 Tue 14:00 Poster B

Spectroscopic investigation of periodic plasmonic superstructures — •Ekaterina Ponomareva and Matthias Karg — Heinrich-Heine-University Düsseldorf, Physical Chemistry I, Düsseldorf, Germany

Nanoparticles with a plasmonic metal core and a soft cross-linked hydrogel shell spontaneously self-assemble at an air/liquid interface forming periodic monolayers [1]. These layers can be transferred on glass substrates yielding substrate-supported superstructures with hexagonally arranged plasmonic nanoparticles at inter-particle distances of a few hundred nm. Due to the spatial proximity and the periodicity of the array, localized surface plasmons of metal cores can couple to diffractive modes and thus support surface lattice plasmon resonances [2]. By embedding the monolayer into a gain-medium these resonances can be enhanced.

Here we will demonstrate the angular-dependent optical behavior of periodic plasmonic monolayers. UV-vis measurements show different optical properties for dilute particles in aqueous dispersion, the assembled monolayers and the monolayers upon embedding in a gain matrix. A home-made lasing-spectrometer was used to investigate the collective optical response of the plasmonic lattices in dependence on the detection and incident angle. With the set-up it is possible to observe the near-field and radiative plasmonic coupling effects in colloidal monolayers.

[1] K. Volk et al., Adv. Mater. 24 (2015), 7332

[2] K. Volk et al., Adv. Optical Mater. 5 (2017), 1600971

CPP 32.7 Tue 14:00 Poster B

Ugi four-component reaction as versatile tool for multifunctional polysaccharide microgel fabrication — •Nicolas Hauck[1], Nalin de Seixas Borges[2], Ludger Wessjohann[2], Andreas Fery[1], and Julian Thiele[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Leibniz-Institut für Pflanzenbiochemie, Halle, Germany

Polysaccharide-based microgels are of special interest in cell biology, tissue engineering, drug delivery, and cell-free biotechnology. However, hydrogel synthesis from polysaccharides often requires prefunctionalization of respective building blocks for subsequent crosslinking as well as for introducing other functionalities. In this context, it is particularly disadvantageous that conventional polymer-analogous coupling reactions often cannot simply be applied on polysaccharides due to an insufficient degree of functionalization. Thus, additional, time-consuming synthesis steps have to be afforded, before polysaccharide-based materials can be processed into defined microgels.

To address these challenges, we utilize multicomponent reactions, which allow for functionalization, e.g. with bioactive compounds or fluorescent dyes, and crosslinking of hydrogel precursors in parallel without time-consuming pre-modifications of precursors. Especially, the Ugi four component reaction is well suited for that purpose. Based on carboxylic acid-rich hyaluronic acid and a diamine as bifunctional crosslinker, hydrogels can be crosslinked with different functional aldehydes and isocyanides in situ to yield multifunctional microgels.

CPP 32.8 Tue 14:00 Poster B

UV-Rheo-Raman: Chemo-mechanical monitoring of UV-cross-linking of polymers — •Moritz Strobel, Robert Gerstmayr, Milan Kracalik, and Sabine Hild — Johannes Kepler University, Institute for Polymer Science, Linz, Austria

Hydrogels are rising up to meet requirements of many different fields and are of increasing interest in various applications, such as soft contact lenses, wound dressing or stretchable electronics. Many studies have focused on the different areas of applications but fewer investigate the connection between mechanical and chemical properties of these polymers and the influence of different curing parameters on the obtained product. In our approach we investigate simultaneously the chemical and mechanical properties at the different stages of curing of the hydrogels. This allows us to recognize correlations between for example the reaction turnovers and the gel point. Aim of this study is to investigate the influence of the intensity and the exposure time of the UV-light initiating the curing process on the obtained hydrogel. Therefore, mechanical properties are obtained by shear rheology measurements analyzing the storage and the loss modulus. An installed UV-laser enables us to perform in-situ rheo-Raman-measurements while curing the hydrogel. Chemical information regarding the cross-linking of the polymers while initiating the curing with UV-light is obtained by adding Raman spectroscopy to this set-up.

CPP 32.9 Tue 14:00 Poster B

Enzymatic synthesis of stimuli-responsive microgels — •Elisabeth Gau[1,2], Franziska Flecken[1,2], Agnieszka Natalia Ksiazkiewicz[1,2], and Andrij Pich[1,2] — [1]DWI - Leibniz-Institute for Interactive Materials e.V., Forckenbeckstraße 50, 52074 Aachen — [2]Functional and Interactive Polymers, Institute of Technical and Macromolecular Chemistry, RWTH Aachen University, Worringerweg 2, 52074 Aachen

Aqueous microgels are highly crosslinked, polymer colloids exhibiting promising properties for many applications in the biomedical field, like softness and stimuli-responsiveness depending on the incorporated monomers.[1,2] The most frequently used method for microgel synthesis is precipitation polymerization. For initiation, mainly thermic initiators like azo- or peroxide-based compounds are used, limiting the possible reactants to thermo stable substances.[2] Enzymatic initiation is a promising alternative to enable the incorporation of thermo instable biomolecules into polymers by decreasing the reaction temperature. Herein, we present the use of a glucose oxidase-based initiator system for the synthesis of aqueous microgels.[3] Glucose oxidase catalyzes the oxidation of β-D-glucose with molecular oxygen to D-glucono-lactone and hydrogen peroxide. Through the addition of ferrous ions (Fe2+), the hydrogen peroxide is cleaved into hydroxyl radicals. These radicals act as initiators for the polymerization reaction.[4]

[1]: Pich et al., Adv. Polym. Sci. 2011, 234, 1-37. [3]: Gau et al., Green Chemistry 2017, accepted. [4]: Johnson et al., Biomacromolecules 2009, 10, 3114-3121.

CPP 32.10 Tue 14:00 Poster B

Expandable and though hydrogels for gel-embodied soft machines — •Robert Gerstmayr[1], Moritz Strobel[1], Daniela Wirthl[2], Robert Pichler[2], Florian Hartmann[2], Sabine Hild[1], Siegfried Bauer[2], and Martin Kaltenbrunner[2] — [1]Institute of Polymer Science-JKU, Linz, Austria — [2]Soft Matter Physics-JKU, Linz, Austria

Natural hydrogel hybrids inspired scientists to develop wide ranging classes of soft hydrogel-based electronic, ionic and photonic devices based on soft and soft-to-hard hybrid architectures. For these applications tough hydrogels have proven to be a superior material due to their high flexibility and adequate strength. The tough gels we produced are full simultaneous interpenetrating polymer double networks, physically interlaced and inseparable. The materials show an advanced flexibility introduced by the energy dissipating reload mechanism of the second network. To obtain a prominent level of complexity a combination of several materials is needed. Which is achieved by bonding several layers consisting of various materials. A challenging task is to overcome the low interfacial toughness when bonding diverse substances to water-rich hydrogels. Cyanoacrylate adhesives, which rapidly polymerize in the presence of hydroxyl groups of water mixed with branched alkanes, form an easy-to-use colloidal glue suspension with tailorable properties. Raman spectroscopy was used for the characterization of the bonding interface. The diffusion behaviour and the thickness of the resulting moisture curing cyanoacrylate adhesive layer were analysed. Cyclic tensile tests were performed to examine the Mullins effect.

CPP 32.11 Tue 14:00 Poster B

The Electrostatic Expansion of Ionic Microgels — Carlos G. Lopez, Thomas Lohmeier, •John E. Wong, and Walter Richtering — RWTH Aachen University

We report dynamic light scattering data for the hydrodynamic radius of a weakly charged PNIPAM based microgel as a function of temperature and added salt concentration.

Incorporation of 2% ionic co-monomers leads to an increase in the volume phase transition temperature of the microgel, which can be partially suppressed by addition of salt.

The charge induced swelling data are interpreted within the framework of the Flory-Rehner model, modified to include a Donnan term to account for the additional osmotic pressure arising from entropy of dissociated counterions. This model strongly under-predicts microgel swelling at all temperatures and added salt concentrations.

Our results suggest that repulsion between charged polymer segments plays a leading role in microgel expansion. Mean field theories for polyelectrolyte gels do not quantitatively capture this feature.

CPP 32.12 Tue 14:00 Poster B

Degradable Microgels by Radical Ring Opening Polymerization (RROP) in Miniemulsion — Larissa Hussmann[1,2] and •Andrij Pich[1,2] — [1]DWI Leibniz Institute for Interactive Materials, Aachen, Germany — [2]RWTH Aachen University, Aachen, Germany

Due to their porous structure, water absorption and swelling capability, microgels have been applied in tissue engineering, release systems and coating devices. Especially Poly (N-vinylcaprolactam) (PVCL) microgels are interesting candidate for application in biomaterials due to their biocompatibility. However, in order to synthesize PVCL microgels that are able to release molecules or degrade in controlled way, degradable units need to be integrated into the microgel structure. In this work we follow a new approach that allows incorporation of degradable units into the PVCL chains of the microgel network. In our approach we focus on the copolymerization of VCL and a cyclic ketene acetal, to incorporate a degradable ester function in the polymer backbone, after radical ring opening polymerization (RROP)[1]. Obtained microgels may be suitable to a variety of bio-medical applications, due to their degradability as well as ability to solubilize hydrophobic molecules [2]. Also by varying the copolymer structure of microgel chains, it is expected to control the volume phase transition temperature (VPTT) and swelling of the microgels in aqueous solutions.

[1] Bailey, W.J., Z. Ni, and S.-R. Wu, Journal of Polymer Science: Polymer Chemistry Edition, 1982. 20(11): p. 3021-3030. [2] Shi, Y. and S. Agarwal, e-Polymers. 2015. p. 217.

CPP 32.13 Tue 14:00 Poster B

Optical properties of FePt-nanoparticle loaded microgels — •Alexander Nedilko[1], Katharina Wiemer[2], Ulrich Simon[2], and Gero von Plessen[1] — [1]Inst. of Physics (IA), RWTH Aachen — [2]Inst. of Inorganic Chemistry, RWTH Aachen

Microgels are polymer networks of micrometer or submicrometer dimensions. Suspended in a liquid, e.g., water, microgels are sensitive to ambient conditions such as temperature or pH. Good biocompatibility makes the microgels particularly interesting due to their potential use for the controlled delivery of drugs or in biotechnology. By loading the microgels with iron-platinum nanoparticles (FePt NPs), which are good absorbers of light in the UV-vis spectral range, it is possible to create hybrid materials with interesting optical properties. The volume phase transition (VPT) of the microgels can be triggered by thermal and photothermal heating. We investigate the optical properties of FePt-NP loaded poly(N-vinylcaprolactam)-based microgels during the volume phase transition. For this purpose, we use an integrating sphere to separate from each other the parts of the incident light that are absorbed and scattered by the hybrid structures. The measurements show that the scattered part experiences a pronounced increase during the VPT of the microgel whereas the absorbed part remains almost at the initial value. The increase of the scattered part is caused by a change in the refractive index of the microgel material that results from the VPT.

CPP 33: Poster Session III

Topics: Wetting and Microfluidics (33.1-33.2), Soft Matter Physics: Emerging Topics, New Instruments and Methods (33.3-33.5), Functional Polymer Hybrids and Composites (33.6-33.12), Complex Fluids and Colloids (33.13-33.23), Confined Liquids (33.24-33.25), Droplets, Waves and Instabilities at Surfaces and Interfaces (33.26-33.28), Responsive and Adaptive Systems (33.29-33.31), Nanostructures, Nanostructuring and Nanosized Soft Matter (33.32-33.42).

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

CPP 33.1 Tue 14:00 Poster C

Microfluidic flow cell design based on additive manufacturing — •Max Männel, Ricardo Bernhardt, Andreas Fery, and Julian Thiele — Leibniz-Institut für Polymerforschung e.V., Dresden, Germany

Droplet-based microfluidics has undergone a rapid growth in recent years due to its potential in material design and biological applications. The most common technique for microfluidic flow cell fabrication is a combination of photo- and soft lithography. In this process, the widely used poly(dimethylsiloxane) (PDMS) is cured to replicate the microchannel structure, which is then bound to a glass slide. This multi-step process is time-consuming and arduous. A promising alternative technique is additive manufacturing utilizing stereolithography (SL). This 3D printing technique has drawn attention due to its low-cost fabrication and fast process time. It is based on a Digital Light Processor (DLP), which translates a digital image into a XY-illumination pattern. This way, a 3D CAD design of a micro flow cell can be printed layer-by-layer.

While the formation of double and higher-order emulsion droplets in planar flow cells generally requires spatially resolved microchannel wettability, we fabricated 3D-printed non-planar microchannels via SL with a resolution of 100 μm for the first time to avoid the influence of wettability. Additionally, 3D-printed planar emulsion generators with a resolution of 20 μm were fabricated. With that, we are able to fabricate micro flow cells with the same resolution as in conventional fabrication methods, but within much shorter process time.

CPP 33.2 Tue 14:00 Poster C

Evolution of invading fluid interfaces at different wetting conditions and pore geometry — •Li weiwei[1,2], Martin Brinkmann[1], Hagen Scholl[1,2], and Ralf Seemann[1,2] — [1]Saarland University, Experimental Physics, D-66123 Saarbrücken, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, D-37077 Göttingen, Germany

Wettability is an important factor that controls the front morphology during displacement of immiscible fluids. With the help of X-ray microtomography, we record the fluid front morphologies emerging during the fluid invasion into random piles of spherical beads. We identified two qualitatively different displacement regimes that are controlled by the advancing contact angle of the invading fluid. For the accurate characterization of the fluid front evolution, we considered several quantities related to the geometry of the interface. Extending our experiments to low contact angles and non-spherical grains, we found displacement patterns that differ substantially from those previously reported for spherical beads packs [1]. This result reveals the combined influence of wetting conditions and pore geometry on the global evolution of the fluid distribution.

[1] K. Singh, H. Scholl, M. Brinkmann, M. DiMichiel, M. Scheel, S. Herminghaus, and R. Seemann. Sci. Rep. 7: 444 (2017).

CPP 33.3 Tue 14:00 Poster C

Density determination of liquids in the pressure range up to 5000 bar — Julia Nase, Miren Büyükasik, Mirko Elbers, Michael Paulus, Paul Salmen, Christian Sternemann, •Göran Surmeier, and Metin Tolan — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany

The knowledge of the density of liquids is of high importance in many fields of research. Densities need to be known e.g., for the exact analysis of Terahertz spectroscopy data or X-ray scattering data. Exact values are also needed to verify theoretical density models and as parameter for Molecular Dynamics simulations of liquids. Densities of liquids are typically measured in a vibrating tube densitometer (VTD) with high accuracy, however limited to a small range of temperature and pressure. Notably, the pressure can be increased to several 100 bar only. From the increasing interest in high hydrostatic pressure conditions in the last years, the need for density data in the kbar regime was arising. We present a setup to determine densities of liquid samples from X-ray absorption measurements at pressures up to 5000 bar. Comparing to numerical simulations and data from a VTD, we show that relative density changes can be determined reliably in the whole pressure range. Trimethylamine-N-oxide, urea, and salt solutions were examined. Experiments were performed at beamline BL8 of DELTA (Dortmund, Germany).

CPP 33.4 Tue 14:00 Poster C

Temperature evolution of the density disturbance in water on attosecond timescale — •Mirko Elbers[1], Nozomu Hiraoka[2], Yury Forov[1], Susanne Dogan[1], Christopher Weis[1], Christian Sternemann[1], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]National Synchrotron Radiation Research Center, 30076 Hsinchu, Taiwan

Water is one of the key components of life on this planet. Its unique properties and anomalies make it highly relevant for many processes in physics, biology and chemistry. In order to investigate those processes, ultrafast techniques such as pump-probe experiments gained in importance during the last years, leading to a better understanding of e.g. the hydrogen bond dynamics in bulk water. We used a different approach, introduced by Abbamonte et al. (Phys. Rev. Lett. 92, 237401, 2004), to image the dynamics of the electron density disturbance in liquid water. This ultrafast imaging method utilizes inelastic x-ray scattering to map the electron density disturbance on an attosecond timescale with an atomic spatial resolution. This is achieved by inverting the energy loss function, accessible in the experiment for a wide range of momentum and energy transfers, into time and space. In this study we take a closer look on the electron dynamics in water at various thermodynamical conditions i.e. different temperatures and pressures, reaching a time resolution below 9 as. The experiments were performed at beamline BL12XU of SPring-8 (Koto, Japan).

CPP 33.5 Tue 14:00 Poster C

Application of adaptive resolution simulations: free energy calculation in liquids and proteins — •Raffaele Fiorentini[1], Aoife Fogarty[1], Raffaello Potestio[2], and Kurt Kremer[1] — [1]Max Planck Institute for Polymers, Mainz, Germany — [2]Department of Physics of the University of Trento, Trento, Italy

A fully atomistic modelling of many biophysical and biochemical processes at biologically relevant length- and time-scales is beyond our reach with current computational resources. One approach to overcome this difficulty is the use of multiscale simulation techniques in which different system components are simultaneously modelled at different levels of resolution. In the case of biomolecules, functionally relevant parts of the system are modelled at as high a level of detail as necessary, while the remainder of the system is represented using less expensive models. Such a multiscale simulation can employ an Adaptive Resolution Simulation (AdResS) methodology, in which the simulation box is divided into atomistic and coarse-grained regions with solvent particles smoothly changing their resolution on-the-fly as they move between regions. In this talk I will discuss how the AdResS approach can be applied to the calculation of thermodynamical properties of biomolecules, and employ it for the first time in combination with Thermodynamic Integration to calculate free energies.

A further multiscale simulation method is the dual resolution approach in which the biomolecule has a dual fixed resolution: atomistic and Coarse Grained part. In this case, the dual-resolution model is employed to compute the protein's free energy landscape.

CPP 33.6 Tue 14:00 Poster C

Soft X-ray analysis of microgels and polymer-based microcontainers in aqueous environment — •Andreas Späth[1], George Tzvetkov[2], Gaio Paradossi[3], and Rainer H. Fink[1] — [1]Friedrich-

Alexander Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II and ICMM, Erlangen, Germany — [2]University of Sofia, Department of Inorganic Chemistry, Sofia, Bulgaria — [3]Universita di Roma Tor Vergata, Dipartimento di Scienze e Tecnologie Chimiche, Rome, Italy

Polymer-based microgel and core-shell particles are versatile containers for the transport of drugs, theranostic gases or catalytically active molecules. They are in many cases biodegradable and fully compatible to in-vivo applications. During recent years we have investigated a broad range of such hybrid materials ranging from gas filled microballoons and thermoresponsible microgel networks to magnetoresponsive particles with embedded iron nanoparticles and core-shell systems filled with theranostic gases or catalytically active fluids. Soft X-ray microscopy is an excellent tool to study those systems in-situ in aqueous matrix with high-resolution and chemical sensitivity. We have analyzed shell thicknesses, swelling behaviors and temperature response to contribute better understanding on release mechanisms and have developed procedures to derive high-resolution 3D representations of the particles from 2D transmission micrographs. The project is funded by the BMBF (05K16WED).

CPP 33.7 Tue 14:00 Poster C

Study on inner structure and carrier dynamics of colloidal quantum dots solids — •Wei Chen and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Colloidal quantum dots (CQDs) have attracted a lot of research interests in both optoelectronics and photovoltaics due to their unique properties, including tunable band-gap, solution processability and the high monodispersity. Due to the intensive investigations on their surface engineering, CQDs based homo-junction solar cells have achieved similar power conversion efficiency (PCE) as compared to top-class bulk heterojunction (BHJ) organic solar cells. The surface engineering is working on not only decreasing the trap states of CQDs* surface, but also optimizing the positions of each CQDs among the array, which is supposed to be the key factor to achieve higher charge mobility. We use inorganic and organic iodide ions sources to proceed the ligands exchanges on the surface of CQDs during the solids forming by spin coating in a layer by layer fashion. We use grazing incidence small angel x-ray scattering to confirm the inner structure changes of the films, including the inner dot spacing and the structures in larger scale, of CQDs solids under different ambient conditions. Moreover, the femtosecond pump-probe transient absorption spectroscopy (TA) is used to study the carrier dynamics of CQDs solids.

CPP 33.8 Tue 14:00 Poster C

Morphology phase diagram of printed titania films derived from block copolymer assisted sol-gel templating — •Nian Li, Bo Su, Senlin Xia, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Printing, a simple and low-cost technique for producing films on an industrial scale, is employed to fabricate mesoporous titania thin films. Titanium(IV)isopropoxide (TTIP) is used as precursor and a diblock copolymer polystyrene-block-polyethylene oxide (PS-b-PEO) as the structure-directing template. The amphiphilic block copolymer PS-b-PEO undergoes phase separation and self-assembly due to a good-bad pair solvent, 1,4-dioxane and hydrochloric acid (HCl), respectively. By adjusting the weight fraction of 1,4-dioxane, HCl and TTIP, the titania films with different morphologies are obtained after evaporation and calcination processes. The surface morphology is probed via scanning electron microscopy (SEM) and atomic force microscopy (AFM), and the inner morphology is detected by grazing incidence small-angle X-ray scattering (GISAXS). A high degree of crystallinity of anatase titania is proved by X-ray diffraction (XRD) through optimizing the calcination temperature. The optical properties are examined with UV/Vis spectroscopy.

CPP 33.9 Tue 14:00 Poster C

Magnetic Nanoparticles in Diblock Copolymer Matrix — •Kalyan Biswas[1], Senlin Xia[1], Sara Lafuerza[2], Pieter Glatzel[2], Matthias Opel[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]ESRF, Grenoble, France — [3]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching

Fabrication of nanostructured films composed of a polymer matrix and inorganic functional nanoparticles is highly desirable due to its interesting physical properties in the areas of magnetic sensors. Hybrid films of the diblock copolymer polystyrene-b-(ethylene oxide) (PS-b-PEO) and surface-functionalized magnetic nanoparticles (Fe3O4 with hydrophobic coating) are prepared via spin coating. Both real-space and reciprocal-space techniques are employed to characterize the obtained nanocomposite films. The micro- and nanostructures of the magnetic films as a function of the nanoparticle concentration are probed using optical microscopy, scanning electron microscopy, atomic force microscopy, and grazing incidence small-angle X-ray scattering (GISAXS). The observed structures are explained in the framework of microphase separation and confinement. By using superconducting quantum interference device (SQUID) magnetometer, the magnetic property of the hybrid films like superparamagnetism is explored. The electronic and magnetic structures of the hybrid films are studied by resonant inelastic X-ray scattering and X-ray magnetic circular dichroism (RIXS-XMCD).

CPP 33.10 Tue 14:00 Poster C

Nanostructured titania templated by amphiphilic diblock copolymer for lithium-ion battery anodes — •Shanshan Yin, Lin Song, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Lithium-ion batteries (LIBs) have been widely used in many aspects of modern life. Compared with conventional graphite anodes, titania possesses higher capacity and better operation safety, which makes it a promising substitute to the commonly used graphite anodes. However, problems such as gradual capacity decay and relative high intercalation potential hinder its practical application. It has been reported that nanostructured titania can efficiently improve the electrochemical performance. Therefore, in this work titania nanostructures are prepared via sol-gel synthesis in combination with the amphiphilic diblock copolymer poly(styrene-block-ethylene oxide) (PS-b-PEO) as structure-directing agent. The morphology of the obtained titania nanostructures is studied with optical microscopy (OM) and scanning electron microscopy (SEM), while the optical properties are investigated with UV/Vis spectroscopy and Photoluminescence (PL).

CPP 33.11 Tue 14:00 Poster C

Orientation of Halloysite nanotubes embedded in a polymer matrix — •Oliver Löhmann[1], Olivier Felix[2], Yuri Lvov[3], Gero Decher[2], and Regine von Klitzing[1] — [1]Technische Universität Darmstadt — [2]Institut Charles Sadron — [3]Louisiana Tech University

Halloysites are inorganic, biocompatible nanotubes consisting of alumosilcates with a length of 0.5 - 2 microns and a diameter of 50 - 80 nm. [1] The surface of the inner lumen is predominated by alumina with a positive surface charge and therefore available for adsorption and protection of small molecules. The nanotubes have an overall negative surface potential at moderate pH due to predomination of silica at the outside. That opens the possibility to embed them into positively charged polyelectrolytes. Zhao et al. showed that Halloysites orientate parallel to each other at the liquid-substrate contact line during solvent evaporation. [2] Based on this we built up multilayers of orientated halloysite over a larger area by controlled spraying method.

Here, we show that halloysites can be orientated by gracing incident spray coating. [3] Multilayers of Halloysites and polyelectrolytes are built up by alternating spray coating. Topology as well as mechanical properties of composites with different layer numbers and compositions measured with Atomic force microscopy will be presented.

[1] Lvov et al., Prog Polym Sci 38 (2013) 1690 - 1719
[2] Zhao et al., J Colloid Interf Sci 440 (2015) 68 - 77
[3] Blell et al., ACS Nano 11 (2017) 84 - 94

CPP 33.12 Tue 14:00 Poster C

Novel Boehmite-embedded organic/inorganic hybrid nanocomposite: cure behaviour, morphology and thermal properties — •Ievgeniia Topolniak[1], Vasile-Dan Hodoroaba[1], Sigrid Benemann[1], Dietmar Pfeifer[2], and Heinz Sturm[1] — [1]Federal Institute for Materials Research and Testing (BAM), Unter den Eichen 87, 12205 Berlin, Germany — [2]Federal Institute for Materials Research and Testing (BAM), Richard-Willstaetter-Strasse 11, 12489 Berlin, Germany

Hybrid materials have attracted growing interest during the last decade, particularly due to their extraordinary properties. Cycloalyphatic-epoxy oligosiloxane (CEO) resin was shown to be a good candidate as a barrier material for the encapsulation purposes. Incorporation of nanoparticles such as Boehmite (BA) into polymers was observed to modify their specific characteristics, in particular, thermal, thermo-oxidative and barrier ones. In this work, novel BA-embedded organic inorganic hybrid nanocomposite material was engineered by combining the advantageous properties of hybrid polymers and nanoparticle enhancement effect. Impacts of particles on the photocuring kinetics, degree of crosslinking and the resultant changes in the thermal properties of the cured films were investigated. CEO synthesis via condensation reaction was confirmed by 1H and 29Si NMR. The particle distribution within the films was verified by SEM including transmission mode coupled with EDX elemental analysis. Photocuring kinetics and thermal properties of the films were studied by in situ FTIR spectroscopy and DSC with TGA, respectively.

CPP 33.13 Tue 14:00 Poster C

Comparison of different measurement techniques for optical contrast factors for ternary mixtures — •Marcel Schraml, Thomas Triller, Roman Reh, and Werner Köhler — Institute of Physics, University of Bayreuth, 95440 Bayreuth, Germany

Non-isothermal diffusion in ternary mixtures is extensively studied both on ground and under microgravity conditions on the Internation Space Station ISS (ESA/Roscosmos, DCMIX3). In most cases are optical, contactless techniques the method of choice. These methods have the disadvantage that the measured data need to be transformed from the refractive index space into the concentration space. Therefore the contrast factor matrix $a_{ij} = (\partial n_i/\partial c_j)_{p,T,c_{k\neq j}}$ has to be inverted. We are using self-designed experiments which are based on refraction or interferometry, because commercial refractometers are not accurate enough or can not provide data in a broad temperature range and at wavelengths covering the entire visible spectrum up to the near IR. On the poster we will explain the difficulty of the contrast factor determination and discuss the different mesurement methods.

CPP 33.14 Tue 14:00 Poster C

Isotropic-nematic phase transition in a 3D lattice model of hard rods with sticky attractions — •Paul Quiring, Miriam Klopotek, and Martin Oettel — University of Tübingen, Germay

We investigate the isotropic-nematic phase transition in a 3D lattice model of 1x1x8-sized hard rods with nearest-neighbor attractions via grand canonical Monte Carlos simulations. It appears that below a critical-like temperature the transition between an isotropic gas state and a nematic liquid state is strongly first order. Above that temperature, the isotropic-nematic transition appears to be weakly first order, as in the corresponding system with no attractions. We also implemented successive umbrella sampling [1] to resolve the transition better. We compare the phase diagram to that calculated with classical Density Functional Theory [2], which overestimates the strength of the transition.

[1] R. L. C. Vink, S. Wolfsheimer, and T. Schilling. Isotropic-nematic interfacial tension of hard and soft rods: Application of advanced grand canonical biased-sampling techniques. The Journal of Chemical Physics, 123(7):074901, 2005.

[2] M. Mortazavifar and M. Oettel. Phase diagrams for sticky rods in bulk and in a monolayer from a lattice free-energy functional for anisotropic particles with depletion attractions. Physical Review E, 96(3), 2017.

CPP 33.15 Tue 14:00 Poster C

A new approach to evaluate the phase gradient in diffusion measurements by digital interferometry — •Daniel Sommermann, Thomas Triller, and Werner Köhler — Institute of Physics, University of Bayreuth, 95440 Bayreuth, Germany

In order to get a better understanding of thermodiffusion in ternary mixtures, the so called DCMIX experiments (Diffusion Coefficients in MIXtures) were performed on the International Space Station (ISS) using the SODI-interferometer (Selective Optical Diagnostics Instrument) under microgravity conditions. This Mach-Zehnder-Interferometer measures the Soret effect by applying a vertical temperature gradient to the system and using digital interferometry with laser phase stepping for readout.

Information about mass diffusion coefficients is obtained by an evaluation of the phase of the interferogram which is done by temporal phase shifting using five pictures in a row. Unfortunately, the readout laser in the DCMIX3 microgravity experiments suffered from instabilities and phase fluctuations. Usual temporal phase shifting algorithms are expecting a constant change in phase and are therefore unable to evaluate part of the data.

In this work a new spatial evaluation methode is introduced which can handle the problem of nonconstant phase stepping by analysing all pictures individually, thereby reconstructing the phase gradient.

CPP 33.16 Tue 14:00 Poster C

Network formation and clustering in a simple Monte Carlo model for protein solutions — •Frank Hirschmann, Marc Habinger, Malte Lütje, Johannes Bleibel, and Martin Oettel — Institut für angewandte Physik - Computational Soft Matter and Nano-Science, Universität Tübingen, Germany

Recent experimental investigations of globular proteins in solutions with three-valent salt ions show interesting phase behavior as well as the formation of extended clusters for a specific parameter range. This can be explained by condensation of salt ions to the surface groups of the proteins, thus leading to aggregation by forming ion bridges via short-range Coulombic attraction.

In order to analyze these results theoretically, we introduce a "patchy particle" model, realized by a non-additive, binary mixture, consisting of hard sphere-like "particles" representing proteins and "floating bonds" representing "bridging ions". By using Brownian-like dynamics simulations, we analyse the emerging network structure and clustering properties both in the spatial and temporal domain.

CPP 33.17 Tue 14:00 Poster C

Halloysite nanotubes surface manipulation by catalyst to control physico-chemical properties of Pickering emulsions — •Sebastian Stock[1], Dmitrij Stehl[1], Regine von Klitzing[1], Yuri Lvov[3], Tobias Pogrzeba[2], and Reinhard Schomäker[2] — [1]TU Darmstadt, Hochschulstraße 6-8, 64289 Darmstadt — [2]TU-Berlin, Straße des 17 Juni 124, 10623 Berlin — [3]Louisiana Tech University, 911 Hergot Ave, Ruston, LA 71272, USA

An emulsion with water and oil has a natural tendency to separate in two phases very fast. The high surface energy is minimized by minimizing the surface between the oil and the water phase. To prevent this process and stabilize the emulsion nanoparticles can be used. Suitable particles for this are the Halloysite nanotubes (HNTs). In opposite to common spherical Nanoparticles HNTs are multiwall tubes based on aluminosilicate. They are around 50 nanometers in diameter and can be up to 1 micrometer long. HNTs have the ability to adsorb at the oil/water interface, change the interface properties this way and stabilize the emulsion. These particle stabilized emulsions are named Pickering emulsions (PEs). Different factors influence the PEs structure. The variation of the PEs HNT and salt (NaCl) concentration and HNT surface modifications by the Rh-catalyst were studied. In order to evaluate the PEs properties, the droplet size and the zeta potential are determined.

CPP 33.18 Tue 14:00 Poster C

Modification of polymer particles with Rh-catalyst for stabilization of Pickering emulsions in catalysis — •Sandra Forg, Dmitrij Stehl, and Regine von Klitzing — Institut für Festkörperphysik, Technische Universität Darmstadt, Alarich-Weiss-Straße 10, D-64287 Darmstadt

Particle stabilized oil-in-water emulsions, so called Pickering emulsions, are useful for many applications, i.e. the liquid/liquid catalysis. To create such emulsions nanoparticles accumulate at the interface of the two liquids to prevent them to coalesce. The benefit of these emulsions is the increase of the surface area available for catalytic reactions, which enhances the efficiency of these reactions. Besides, the stabilized Pickering emulsions should make it easier to recover the catalyst.

Due to this reason, emulsions stabilized both with Poly(N-isopropylacrylamide) (PNIPAM) and with Polystyrene-NH2 (PS-NH2) will be used during this work. Both particles will have a positive charge and thus, the negatively charged Rh-catalyst will adsorb on them. By modification of the ratio between particles and catalyst, the hydrophobicity will be changed. Furthermore, PNIPAM has the benefit that it is temperature-responsive. Due to this temperature-dependence, the diameter of PNIPAM and its chemical affinity to water can be easily affected by changing the temperature. This will result in changes in the stability of the emulsion. A main goal of this work will also be the improvement of knowledge of Pickering emulsions with respect of different properties such as their stability, their structure or the immobilization of the catalyst on the particles.

CPP 33.19 Tue 14:00 Poster C

Structure properties of biaxial phases formed by mixtures composed of uniaxial liquid crystal particles. — Robert Skut-

nik, •Louis Lehmann, Sergej Püschel-Schlotthauer, and Martin Schoen — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Sekr. C7, Straße des 17. Juni 135, Berlin 10623, Germany

Liquid crystals consist of organic molecules of anisotropic shapes. With respect to their shape, they can be classified as disc- and rod-like particles. Both types of particles undergo an isotropic-nematic phase transition. In the nematic phase, the particles align parallel to each other and exhibit thereby a long-range orientational order. In mixtures of discotics and rods, the favored configuration of two separate disc-like particles or two rod-like particles remains parallel. However, rod-like particles align perpendicularly to the disc-like particles with respect to their symmetry axes. In order to study the phase transition of such mixtures, we perform isothermal-isobaric Monte Carlo simulations where the interparticle interactions are modeled by an orientation-dependent Lennard-Jones potential. Here we present a phase diagram of a binary mixture including a biaxial nematic phase as well as a mixture of a uniaxial nematic phase and an isotropic phase with reduced degrees of freedom. We use finite-size scaling theory to identify the phase transition temperatures and use different order parameters to analyze the structure of the mixture.

CPP 33.20 Tue 14:00 Poster C

Defect topologies in chiral liquid crystals confined to spherically symmetric cavities — •Robert Skutnik, Sergej Püschel-Schlotthauer, and Martin Schoen — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Sekr. C7, Straße des 17. Juni 135, Berlin 10623, Germany

Liquid crystals exhibit an orientational long range order whereas the positional order remains short ranged. The orientational order of achiral liquid crystals can be described by global quantities. For instance, the the molecules align with their symmetry axes along the global director $\hat{\boldsymbol{n}}$. In chiral liquid crystals the orientational order becomes local and is given by the local directorfield $\hat{\boldsymbol{n}}(\boldsymbol{r})$. Particularly, chiral Blue Phases attract the interest of the scientific community because their orientational distribution appears to be isotropic on a macroscopic length scale whereas regular orientational order is found locally. These properties provide an application as tunable photonic devices. This raises the question for the manipulation of blue phases by external fields (i. e., electromagnetic fields or confinement). Here, we focus on the case of a Blue Phase II confined to a spherical cavity. In order to investigate properties of confined Blue Phases, we perform Monte Carlo simulations in the grand canonical ensemble. The chiral liquid crystal is modeled by a modified 12-6 Lennard-Jones potential which has been repeatedly used to model all known chiral phases adequately. Depending on the cavity diameter as well as on the local alignment at the interface we observe a zoo of novel topological disclination networks.

CPP 33.21 Tue 14:00 Poster C

Entanglement in semiflexible polyelectrolyte solutions — •Carlos Lopez — RWTH Aachen University

We present shear rheology data for solutions of semiflexible polyelectrolyte sodium carboxymethyl cellulose (NaCMC) in salt-free water and aqueous solutions of various electrolytes.

The plateau modulus (G_e), estimated from the crossover between the elastic modulus and loss modulus in oscillatory shear, scales as with concentration $G_e \sim c^{1.7}$. The entanglement concentration is approximately independent of added salt concentration. The data presented here, along with a review of the literature suggests that electrostatics have only a weak effect on entanglements, despite having a large effect on polymer conformation.

The reptation model correctly predicts the variation of solution viscosities with concentration and molecular weight in high salt solution but fails in salt-free solution, where an exponent $\simeq \times 3$ larger than the reptation prediction is observed.

These observations presented here clash with scaling arguments which assume that the entanglement tube diameter is proportional to the correlation length and hence dependent on solvent quality.

CPP 33.22 Tue 14:00 Poster C

Non-Equilibrium States of Sticky Colloidal Particles: Phase Separation and Dynamical Arrest — •Jan Hansen, Carolyn J. Moll, Florian Platten, and Stefan U. Egelhaaf — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Soft materials can form amorphous solids, e.g. gels and glasses, which are relevant for such diverse fields as food engineering, pharmaceutical industry and materials science. To analyze the non-equilibrium states of colloidal particles interacting via short-ranged attractions, we use a perfectly monodisperse suspension of nearly spherical particles, namely globular proteins (lysozyme). The metastable gas-liquid binodal, the attractive glass line and the second virial coefficient B_2 for various solution conditions, i.e. salt concentrations, have been determined by optical microscopy, centrifugation experiments and light scattering. If the temperature axis of the binodals is expressed in terms of B_2, data obtained under various conditions fall onto a master curve, as suggested by the corresponding states law. For colloids with short-ranged attractions, gelation has previously been related to gas-liquid phase separation and a universal state diagram has been proposed if scaled by B_2. However, this is in contrast to our findings. Arrest lines for different salt concentrations overlap within experimental errors, whereas they do not overlap if the temperature axis is replaced by B_2. This indicates that the binodals are not sensitive to the details of the potential, but can be described by one integral parameter, i.e. B_2, whereas the arrest line appears governed by its attractive part.

CPP 33.23 Tue 14:00 Poster C

Pressure-induced phase separation in silica nanoparticle-polymer solutions — •Marc Moron, Julian Schulze, Julia Nase, Michael Paulus, and Metin Tolan — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany

Nanoparticles are in the focus of current research because they are important for many applications like e.g. thermal energy storage or in medical chemistry for gene delivery. Silica nanoparticles in aqueous solution show a repulsive interaction. By adding small non-adsorbing polymers (e.g. polyethylene glycol), the total particle-particle interaction can become attractive. With increasing polymer concentration, the system undergoes a liquid-liquid phase separation. Further increase of the PEG concentration leads to a homogenous solution, which is explained by the repulsive interaction between the polymers. This concentration-dependent phase transition can also be achieved by exposing the system to high pressure. However, a complete understanding of the effect of pressure on the nanoparticle-polymer system is still missing. In this work light transmission and small-angle X-ray scattering (SAXS) measurements are performed, to study systematically the effect of hydrostatic pressure, the molecular weight of PEG and the sample environment on the phase behavior. In that way a complete picture of the system is obtained and the understanding of the phase transition on a microscopic level is increased.

CPP 33.24 Tue 14:00 Poster C

Collective Orientational Order and Phase Behavior of a Discotic Liquid Crystal under Confinement — •Arda Yildirim[1], Kathrin Sentker[2], Patrick Huber[2], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — [2]Institut für Materialphysik und -technologie, Technische Universität Hamburg, Eißendorfer Str. 42, 21073 Hamburg, Germany

Discotic liquid crystals (DLCs) are a promising class of soft matter for electronic applications. This is due to their ability to self-organize into columns in a hexagonal columnar mesophase, driven by the overlapping of the π orbitals of their aromatic cores. This leads to a high charge-carrier mobility along the column axis. Previous studies on DLCs showed that their properties, such as phase transition temperatures and enthalpies, are susceptible to nanoconfinement [1,2]. In this study, 2,3,6,7,10,11 hexakis[hexyloxy] triphenylene (HAT6) was confined into parallel aligned cylindrical nanopores of anodic aluminum oxide (AAO) membranes by melt infiltration. Furthermore, the pore surfaces of a series of membranes were chemically modified, resulting in a more hydrophobic pore surface than the unmodified ones. Collective orientational order and phase behavior of HAT6 confined into modified and unmodified nanopores of AAO were investigated by broadband dielectric spectroscopy and differential scanning calorimetry respectively.
[1] C. Krause and A. Schönhals, J. Phys. Chem. C, 2013, 117, 19712.
[2] C. Krause et al., Colloid Polym. Sci., 2014, 292, 1949.

CPP 33.25 Tue 14:00 Poster C

Static properties of confined hard-sphere fluids — •Lukas Schrack and Thomas Franosch — Institut für Theoretische Physik, Leopold-Franzens-Universität, Technikerstraße 21A, 6020 Innsbruck, Austria

We investigate static properties in a strongly confined hard-sphere liquid between two parallel flat walls. For this purpose, the Ornstein-Zernike integral equation using Percus-Yevick closure relation is solved numerically. The theory requires the density profile perpendicular to the plates as input, which can be obtained from density functional theory. The resulting convolution integral is most efficiently solved by a Fast Hankel transform of zeroth-order with a logarithmically spaced grid yielding to an algebraic equation.

The confinement induces a modulation of the equilibrium density profile with plane waves as the suitable eigenmodes for the planar geometry. We try to solve the inhomogenous Ornstein-Zernike equation in mode representation and compare our results to the calculated Fourier decomposition of the direct correlation function and the static structure factor obtained from the real-space solution.

CPP 33.26 Tue 14:00 Poster C

Cusp-Shaped Elastic Creases and Furrows — •Stefan Karpitschka[1,2], Jens Eggers[3], Anupam Pandey[1], and Jacco H. Snoeijer[1,4] — [1]Physics of Fluids Group, Faculty of Science and Technology, University of Twente, Enschede, Netherlands — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [3]School of Mathematics, University of Bristol, United Kingdom — [4]Mesoscopic Transport Phenomena, Eindhoven University of Technology, Netherlands

The surfaces of growing biological tissues, swelling gels, and compressed rubbers do not remain smooth, but frequently exhibit highly localized inward folds. In biology, such elastic structures are called sulci, which are prime morphological features of human brains and growing tumors. Yet in spite of their ubiquity and importance, a quantitative theoretical description of the morphology of localized indentations is still missing. We reveal the morphology of this surface folding in a novel experimental setup, which permits us to deform the surface of a soft gel in a controlled fashion [Phys. Rev. Lett. 119, 198001 (2017)]. The interface first forms an increasingly sharp furrow. Above a critical deformation, the furrow bifurcates to an inward folded crease of vanishing tip size. We show experimentally and numerically that both creases and furrows exhibit a universal cusp shape, whose width scales like $y^{3/2}$ at a distance y from the tip. We provide a similarity theory that captures the singular profiles before and after the self-folding bifurcation, and derive the length of the fold from finite deformation elasticity.

CPP 33.27 Tue 14:00 Poster C

Spheroidal and conical shapes of ferrofluid-filled capsules in magnetic fields — •Christian Wischnewski and Jan Kierfeld — Department of Physics, Technische Universität Dortmund, 44221 Dortmund, Germany

We investigate the deformation of soft spherical elastic capsules filled with a ferrofluid in external uniform magnetic fields at fixed volume by a combination of numerical and analytical approaches. We develop a numerical iterative solution strategy based on nonlinear elastic shape equations to calculate the stretched capsule shape numerically and a coupled finite element and boundary element method to solve the corresponding magnetostatic problem, and employ different analytical approximations. The observed deformation behavior is qualitatively similar to the deformation of ferrofluid droplets in uniform magnetic fields. Homogeneous magnetic fields elongate the capsule, and a discontinuous shape transition from a spheroidal shape to a conical shape takes place at a critical field strength. We investigate how capsule elasticity modifies this hysteretic shape transition and show that conical capsule shapes are possible but involve diverging stretch factors at the tips, which gives rise to rupture for real capsule materials. At small fields capsules remain spheroidal, and we characterize the deformation of spheroidal capsules both analytically and numerically. Our results can be helpful in order to quantitatively determine capsule or ferrofluid material properties from magnetic deformation experiments. All results also apply to elastic capsules filled with a dielectric liquid in an external uniform electric field.

CPP 33.28 Tue 14:00 Poster C

Beyond the standard line tension: Size-dependent contact angles of water nanodroplets — •Matej Kanduc — Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D-14109 Berlin, Germany

The dependence of the contact angle on the size of a nanoscopic droplet residing on a flat substrate is traditionally ascribed solely to line tension. Other contributions, stemming from the droplet geometry dependence of the surface tension and line tension, are typically ignored. We performed molecular dynamics simulations of water droplets of cylindrical morphology on surfaces of a wide range of polarities. In the cylindrical geometry, where the line tension is not operative directly, we found significant contact angle dependence on the droplet size [1]. The effect is most pronounced on hydrophilic surfaces, with the contact angle increase of up to 10° with a decreasing droplet size. On hydrophobic surfaces, the trend is reversed and considerably weaker. Our analysis suggests that these effects can be attributed to the Tolman correction due to the curved water-vapor interface and to a generalized line tension that possesses a contact angle dependence. The latter is operative also in the cylindrical geometry and yields a comparable contribution to the contact angle as the line tension itself in case of spherical droplets.

[1] M. Kanduc, J. Chem. Phys. 147, 174701 (2017)

CPP 33.29 Tue 14:00 Poster C

Solvation effects and self-organization of a multi-azobenzene photochromic system in aqueous and DMSO/water solutions — •Markus Koch[1], Anastasia B. Danilova[2], Aleksandr S. Pavlov[2], and Olga Guskova[1] — [1]Institute Theory of Polymers, IPF Dresden, Germany — [2]Department of Physical Chemistry, Faculty of Chemistry and Technology, Tver State University, Russia

The star-shaped molecules with benzene-1,3,5-tricarboxamide center (playing a role of gelator) and three photo-sensitive azobenzene arms were found to self-assemble into supramolecular columnar phases in solution [1]. Upon UV-light stimulus, when azobenzenes are isomerized from a planar trans- to a bent cis-state, these aggregates undergo order/disorder transition, which was largely attributed to the changes in molecular geometry. In this work, the concentrated solutions of multi-azobenzene photochromic system [2] in water and DMSO/water mixture are studied at Ångström resolution using all-atom MD simulations aiming at further understanding of the self-assembly and disassembly triggered by light. Comparing the solvation properties of the stars in water and DMSO/water mixtures, we conclude about possible impact of DMSO molecules on the structural properties of the star. Our results represent a useful conceptual starting point to deeper understanding of the experimentally observed morphological transitions triggered by light and upon exposure of columnar phases to pure DMSO.

This work was supported by DFG (Project No GU 1510/3-1).

[1] S. Lee et al. Langmuir 2013, 29, 5869.

[2] M. Koch et al. J. Phys. Chem. B 2017, 121, 8854.

CPP 33.30 Tue 14:00 Poster C

Responsive Copolymer-Graphene Oxide Hybrid Microspheres with Improved Drug Release Kinetic — •Izabela Firkowska-Boden[1], Fuping Dong[1,2], Matthias M. L. Arras[1,3], and Klaus. D. Jandt[1,4] — [1]Chair of Materials Science, Otto Schott Institute of Materials Research, Faculty of Physics and Astronomy, Friedrich-Schiller-University Jena, Löbdergraben 32, 07743 Jena, Germany — [2]Department of Polymer Materials and Engineering, College of Materials and Metallurgy, Guizhou University, Guiyang, 550025, China — [3]Oak Ridge National Lab, Biology and Soft Matter Division, Oak Ridge, TN 37831, USA — [4]Jena Center for Soft Matter (ICSM), Friedrich-Schiller-University Jena, Philosophenweg 7, 07743 Jena, Germany

Polymeric hollow spheres with sizes ranging from the nanometer to the micrometer scale are particularly functional materials owing to their potential application as drug delivery system. In order to control the encapsulation and releasing of drug molecules from the interiors under physiological conditions, smart hollow spheres, which are sensitive to temperature have been reported. In this study we aimed to integrate both high loading efficiency and controlled drug release into a hybrid composite material composed of thermoresponsive copolymer hollow microspheres poly(N-isopropylacrylamide-co-styrene) (PNIPAAm-co-PS) and outer graphene oxide layer. The diffusion-driven drug release is controlled by the electrostatically deposited layer of GO nanosheets, which effectively suppresses the initial burst release and enables sustained drug release in in vitro testing.

CPP 33.31 Tue 14:00 Poster C

Mechano-Responsive Polymer Structures for Sensing Forces — •Jens W. Neubauer[1], Nicolas Hauck[1], Julian Thiele[1], and Andreas Fery[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [2]Chair of Physical Chemistry of Polymeric Materials, Technische Universität Dresden, Germany

We design mechano-responsive polymer structures for spatially resolved force sensing. Local deformations of the polymer cause localized changes in the fluorescence of labelled dyes. Hence, the deformations can be correlated with the mechanical properties of the polymer structure.

Recently, we applied a mechano-responsive polyelectrolyte brush to resolve the stress distributions in the contact area of gecko-inspired microstructures. The polyelectrolyte brush carried permanent cationic charges which could quench the fluorescence of the labelled dye. Accordingly, compressive and tensile stresses could be read out from locally decreased and increased fluorescence intensity, respectively. In earlier work, the sensitivity upon compression was determined to 10 kPa with a spatial resolution better than human skin (1 μm).

As the polymer brush layers are limited in geometry, we aim for extending the responsiveness to three-dimensional polymer networks. For this purpose, we utilize droplet microfluidics.

Neubauer, J. W. *et al. ACS Appl. Mater. Interfaces* **8** (2016) 17870.

Bünsow, J. *et al. Angew. Chem. Int. Ed.* **50** (2011) 9629.

Heida, T. *et al. Macromol. Chem. Phys.* **218** (2017) 1600418.

CPP 33.32 Tue 14:00 Poster C

Polymer structure formation in ITPC foils studied by SAXS — •Ann-Kathrin Grefe, Björn Kuttich, and Bernd Stühn — Institut für Festkörperphysik, Technische Universität Darmstadt

Nanopores obtained by etching of heavy ion irradiated polycarbonate foils present ideal systems for studying polymer structure formation under confinement. Their perfect cylindrical geometry, strict orientation perpendicular to the surface and random lateral distribution allow for an straightforward investigation via small angle x-ray scattering [1].

Polycarbonate foils with pore radii ranging from 17 nm to 59 nm are prepared and characterized via SAXS. The dependency of the pore radius and its polydispersity on the etching time are examined. Subsequent coating of the pores with 10 nm of SiO_2 via atomic layer deposition is shown to result in a well-defined and homogenous surface which does not alter the cylindrical form of the pores.

Two different polymer systems are introduced into the pores via melt infiltration: For a bulk cylinder forming PS-b-PI diblock copolymer in situ SAXS measurements confirm that a nearly complete filling of the pores with polymer can be achieved and a full profile fit can be used to directly monitor the filling kinetics. However, the scattering curves show no indications for a structure formation of the polymer inside the pores. For a PEG homopolymer with a semi-crystalline lamellar structure in bulk the filling process is too fast to be resolved via SAXS. But here changes in the scattering curves of pores with a diameter over 100 nm hint at a structure formation due to partial crystallization.

[1] M. Engel et al., Appl Phys A 97, 99-108 (2009)

CPP 33.33 Tue 14:00 Poster C

Molecular AC electrokinetics using interdigitated electrodes — •Eva-Maria Laux[1], Christian Wenger[2], Frank F. Bier[1], and Ralph Hölzel[1] — [1]Fraunhofer IZI-BB, Potsdam, Germany — [2]IHP GmbH - Leibniz Institute for Innovative Microelectronics, Frankfurt (Oder), Germany

Electrokinetic effects are universally applicable to particles regardless of their charge and - in principle - of their size. However, as a consequence of the interference of thermal motion, a successful manipulation of particles in the nanometer range calls for increasingly high electric field gradients. These can be produced by further miniaturized electrode structures, Here we use interdigitated nanoelectrodes made of tungsten, embedded in silicon dioxide, fabricated on a silicon substrate. Whilst the electrode width and gap width are 750 nm and 450 nm, respectively, the thickness amounts to 100 nm and the curvature of the electrode edges - which is the decisive parameter for dielectrophoretic action - is below 50 nm.

Using these electrodes, we attracted fluorescent proteins (eGFP) to the electrodes and achieved immobilization as well as alignment of the protein molecules. With its cylindric shape with 2.4 nm diameter and 4.2 nm height, eGFP belongs to the smallest objects manipulated by AC electrokinetics up to date. We are pushing this limit further by handling, as an example, the fluorescence dye rhodamine 6G, which has a diameter of approx. 1 nm. The dye molecules are indeed attracted towards the electrode structures and accumulated in the electrode gaps as revealed by fluorescence microscopy.

CPP 33.34 Tue 14:00 Poster C

AC field assisted deposition of antibodies for virus detection — •Sandra Stanke[1,2], Christian Wenger[3], Frank Bier[1,2], and Ralph Hoelzel[1] — [1]Fraunhofer Institute for Cell Therapy and Immunology, Branch Bioanalysis and Bioprocesses IZI-BB, Potsdam, Germany — [2]University of Potsdam, Germany — [3]IHP GmbH, Leibniz Institute for Innovative Microelectronics, Frankfurt/Oder, Germany

Alternating current (AC) electrokinetics is a set of different effects that can be used for the manipulation of nano-particles in a non-uniform electric field. Here, we present an AC-electrokinetic driven sensor for the manipulation and movement of biological nanoparticles. This sensor consists of four individual arrays, each built up of more than 6000 nano-electrodes with a diameter of 500 nm each. Individually controlled functionalization of the sub-arrays is performed by AC electrokinetic forces: dielectrophoresis and AC electroosmosis. Consequently, molecules like antibodies can be attracted to the electrode surface. This allows the local concentration of the analyte at the sensor surface. Since these arrays can be addressed individually, each array can be functionalized with a different antibody. Thus, it is possible to detect, characterize and subtype different strains of the influenza virus. Additionally, each electrode is part of an on-chip resonant circuit, whose frequency changes with surface coverage of the electrode and, hence, serves as a measure of the amount of viruses bound to the antibody. The universal chip design does not limit the application to influenza viruses but also to different viruses, bacteria and parasites.

CPP 33.35 Tue 14:00 Poster C

Evolution of atomic structure and nanoparticle formation during spray deposition of metal organic decomposition inks — •Björn Fricke[1], Wiebke Ohm[1], Calvin Brett[1,2], Matthias Schwartzkopff[1], André Rothkirch[1], Tim Laarmann[1,3], and Stephan V. Roth[1,4] — [1]Deutsches Elektronen-Synchrotron Hamburg, Notkestraße 85, 22607 Hamburg — [2]KTH Royal Institute of Technology, Department of Mechanics, Teknikringen 8, SE-100 44 Stockholm, Sweden — [3]The Hamburg Centre for Ultrafast Imaging CUI, Luruper Chaussee 149, Hamburg 22761, Germany — [4]KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, Teknikringen 56-58, SE-100 44 Stockholm, Sweden

We present a spray deposition process for fabrication of nanostructured silver layers which is advantageous in comparison to other methods. Silver nitrate solution was used as precursor for the nanostructures, which is beneficial, because of its solubility and the low toxicity. We investigated the growth of deposited silver nitrate nanoparticles as well as the influence of an annealing process, by optical and atomic force microscopy and UV-VIS spectroscopy. In addition, in situ GISAXS and GIWAXS were used to identify morphological and chemical changes during the spraying/heating process: The nanoparticle growth was investigated as a function of the spray duration. During the heat-induced transformation, the nanoparticles show coalescence, resulting in a larger percentage of surface coverage in comparison to the as deposited films. Additionally, the temperature dependent conversion from silver nitrate to silver is shown.

CPP 33.36 Tue 14:00 Poster C

Application of the Microfluid Segment Technology for the Preparation of Noble Metal Nanoparticles — •Andrea Knauer and J. Michael Köhler — Technische Universität Ilmenau, FG Physikalische Chemie/Mikroreaktionstechnik, Prof.-Schmidt-Str. 26, 98693 Ilmenau, Deutschland

The microfluid segment technology allows the realization of fast mixing processes and thus a very narrow residence time distribution. This enables optimum preconditions for a fast nanoparticle nucleation and opens up the possibility to generate nanoparticles with highly homogeneous shapes and compositions, narrow particle diameter distributions, and thus pronounced sharp absorption bands in optical spectroscopy. Therefore, a microfluid segment based technique was used for the generation of noble metal nanoparticles. Within this work, microfluidically processed Au/Ag core/shell nanoparticles, triangular silver nanoprisms, silver nanoprisms with a gold shell, or gold nanoframes, and single crystalline gold nanocubes are presented as model systems. By choosing the appropriate reactant ratios, the nanoparticles sizes and thus their optical properties can be tuned with a fine resolution. Depending on size, shape and composition, the spectral position of the absorption maximum can be shifted between 390 and 1000 nm.

CPP 33.37 Tue 14:00 Poster C

How do amino acids behave in intercalation compounds? — •Robby Büchner[1], Annette Pietzsch[1], and István Pálinkó[2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [2]University of Szeged, Hungary

The first soft X-ray spectra of a Layered Double Hydroxide (LDH) and intercalated amino acids are presented. LDHs are clay minerals with the ability to store arbitrary anionic guest species between their positively charged layers. This property enables numerous applications ranging from environmental remediation, to controlled drug delivery and even gene transfer. In order to systematically develop and improve these applications, a profound understanding of the host-guest interactions is essential. Therefore, near-edge X-ray absorption fine structure (NEXAFS) and resonant inelastic X-ray scattering (RIXS) measurements were carried out. They confirmed the widely assumed Coulomb attraction between the LDH host and the guest ions. Additionally, an at least partially covalent bond between the host layers and the amino acids can be stated.

CPP 33.38 Tue 14:00 Poster C

Gold Nanoparticle Growth on Homopolymer Thin Films — •Susann Frenzke[1], Matthias Schwartzkopf[2], Pallavi Pandit[2], Wiebke Ohm[2], Marc Gensch[2], Bjoern Fricke[2], Calvin Brett[2,3], and Stephan V. Roth[2,4] — [1]FernUniversität in Hagen, Universitätsstr. 1, D-58097 Hagen — [2]DESY, Notkestr. 85, D-22607 Hamburg — [3]KTH Royal Institute of Technology, Department of Mechanics, Teknikringen 8, SE-10044 Stockholm — [4]KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, Teknikringen 56-58, SE-10044 Stockholm

Nanostructured noble metal films on polymer layers are of fundamental importance in the field of organic electronics. Moreover, such material combinations have gained importance for stabilizing thin polymer films. We combine sputter deposition with grazing incidence X-ray scattering (GIXS) to investigate in situ [1,2] the growth kinetics of Gold (Au) on polystyrene (PS). We therefore analyze quantitatively the Au nanoparticle layer growth such films and correlate the change in optical properties of the Au/PS system with the thickness of the gold-capped PS layer. Optical measurement methods such as UV-Vis spectroscopy or imaging ellipsometry were employed.

[1] Schwartzkopf, Roth, Nanomaterials 6, 239 (2016).

[2] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015).

CPP 33.39 Tue 14:00 Poster C

Tailoring thermal properties of biodegradable polyester based nanoparticles for drug delivery — •Christian Helbing[1], Damiano Bandelli[2,3], Christine Weber[2,3], Ulrich S. Schubert[2,3], and Klaus D. Jandt[1,3] — [1]Chair of Materials Science, Otto-Schott-Institute of Materials Research, Friedrich Schiller University Jena, Germany — [2]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Germany — [3]Jena Center for Soft Matter (JCSM), Friedrich Schiller University Jena, Germany

According to literature reports, the thermal properties of biodegradable polyesters influence their degradation and hence the release kinetics of actives from corresponding nanoparticles (NP). However, factors such as the hydrophilic / hydrophobic balance (HHB) and the drug loading impact release kinetics as well. We therefore tailor-made polyester based NPs with different thermal properties but constant HHB and size, as confirmed by means of dynamic light scattering and scanning electron microscopy. The NP are composed of a) poly(ϵ-caprolactone), b) block and c) gradient copolymers of δ-valerolactone and δ-decalactone. Differential scanning calorimetry measurements revealed semicrystalline materials with a significantly lowered melting temperature and degree of crystallinity of P(VL-grad-DL). Atomic force microscopy revealed that the NP stiffness correlates with the degree of crystallinity of the used polymer. This work is part of the Collaborative Research Center 1278 "Polytarget: Polymer-based nanoparticle libraries for targeted anti-inflammatory strategies" which is funded by the DFG.

CPP 33.40 Tue 14:00 Poster C

Directed self-assembly supported by laser interference lithography of plasmonic particles for high optical quality application. — •Vaibhav Gupta[1], Patrick T. Probst[1], Andreas Fery[1,2], and Tobias A. F. König[1,2] — [1]Leibniz-Institut für Polymerforschung, e.V., Hohe Str. 6, 01069 Dresden, Germany — [2]Cluster of Excellence Centre for Advancing Electronics Dresden, Mommsen Str. 4, D-01062 Dresden, Germany

Selective arrangement of nanoparticles with predetermined nanometer-scale accuracy is crucial to exploit the collective properties of the resulting assemblies, in particular for photonic and electro-optical nano devices. Here, we fabricate topographically patterned templates comprised of laser interference lithography and soft molding to achieve control over position and interparticle distance of the plasmonic building block. We are able to produce 2D square lattice of gold nanoparticles on a centimeter-scale substrate with cost-effective and up-scalable method. Finally, we prove our results using finite-difference time domain simulation and discuss the tunability of the generated surface lattice resonance(SLR), which is correlated to fill factor 0.8.

CPP 33.41 Tue 14:00 Poster C

Effect of C60 on the Morphology of Strongly Segregated ABC Miktoarm Terpolymers — •Matthias M.L. Arras[1], Hyeyoung Kim[2], Monojoy Goswami[1], Hong Kunlun[1], Bobby G. Sumpter[1], Thomas P. Russell[2,3], and Gregory S. Smith[1] — [1]Oak Ridge National Lab, Oak Ridge, USA — [2]University of Massachusetts Amherst, USA — [3]Lawrence Berkeley National Lab, Berkeley, USA

We investigated the effect of C60 nanoparticles on a series of poly(styrene), poly(isoprene), poly(2-vinylpyridine) (PS-PI-P2VP) miktoarms by small angle scattering. To this end, we synthesized PS-PI-P2VP with symmetric PS and PI blocks and varied the degree of polymerization for P2VP. We denote the ratio between the volume fraction of P2VP and PS (or PI) as α. C60 addition leads to a reduction in the repeat period due, more than likely, to chain relaxation of the arms of the miktoarm terpolymer, in the hierarchical lamellar microdomain morphology (HLM) which forms for $\alpha > 2$. In contrast, in a sample with a tessellated morphology (TM) at short P2VP chains ($\alpha < 1$), we find the opposite behavior, and the repeat period expands dramatically. We explain these distinct differences with the stability of the HLM (observed for $2 > \alpha > 4$) which is robust and insensitve to configurational changes. In contrast, at all-symmetric conditions $\alpha = 1$ and below $\alpha < 1$ many TMs in close proximity are reported which means the morphology is susceptible to changes.

This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by ORNL. HK & TR were supported by AFOSR (16RT1602) and ARO (W911NF-17-1-0003).

CPP 33.42 Tue 14:00 Poster C

Miktoarm Star Terpolymer PS-PI-P2VP Investigated by Small Angle Neutron Scattering — •Matthias M.L. Arras[1], Hyeyoung Kim[2], Jyoti P. Mahalik[1], Weiyu Wang[1], Hong Kunlun[1], Bobby G. Sumpter[1], Thomas P. Russell[2,3], and Gregory S. Smith[1] — [1]Oak Ridge National Lab, Oak Ridge, USA — [2]University of Massachusetts Amherst, USA — [3]Lawrence Berkeley National Lab, Berkeley, USA

We are reporting on the structure of a strongly segregated asymmetric ABC miktoarm terpolymer, PS-*arm*-PI-*arm*-P2VP (SIV), which as determined by small angle neutron or X-ray scattering and transmission electron microscopy. We synthesized fully protonated and partially deuterated SIV miktoarm stars of similar composition where the majority component P2VP is approximately four times the molar mass of the PI or PS block. The results were compared to self-consistent field theory calculations which predicted two possible energy-minimized structures. The most consistent of the two structures was an hierarchical lamellae structure, consisting of lamellae in lamellae. This talk will highlight, that with increasing complexity in polymer architecture, one characterization technique will not necessarily be sufficient for the determination of the structure. A brief discussion of the prospects for resonant soft X-ray scattering in these systems will also be given.

This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by ORNL. HK & TR were supported by AFOSR (16RT1602) and ARO (W911NF-17-1-0003).

CPP 34: Condensed Matter Simulations augmented by Advanced Statistical Methodologies II (joint session DY/CPP)

Time: Tuesday 14:00–15:15 Location: BH-N 128

CPP 34.1 Tue 14:00 BH-N 128

Nonlinear Network description for many-body quantum systems in continuous space — •Markus Holzmann[1], Michele Ruggeri[2], and Saverio Moroni[3] — [1]LPMMC, UMR 5493 of CNRS, Université Grenoble Alpes, F-38100 Grenoble France — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [3]DEMOCRITOS National Simulation Center, Istituto Officina dei Materiali del CNR and SISSA, Via Bonomea 265, I-34136 Trieste, Italy

We show that the recently introduced iterative backflow renormalization [1] can be interpreted as a general neural network in continuum space with non-linear functions in the hidden units [2]. We use this wave function within Variational Monte Carlo for fermionic and bosonic liquid helium in two and three dimensions, where we typically find a tenfold increase in accuracy over currently used wave functions. For two dimensional 4 He, we also show that the iterative backflow wave function can describe both the liquid and the solid phase with the same functional form - a feature shared with the Shadow Wave Function, but now joined by much higher accuracy.

[1] M. Taddei, M. Ruggeri, S. Moroni, and M. Holzmann, Phys. Rev. B 91, 115106 (2015).

[2] M. Ruggeri, S. Moroni, and M. Holzmann, cond-mat/1711.01993 (2017).

CPP 34.2 Tue 14:15 BH-N 128

Massively parallel multicanonical simulations — Jonathan Gross[1], •Johannes Zierenberg[2], Martin Weigel[3], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Postfach 100920, D 04009 Leipzig, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen, Germany, — [3]Applied Mathematics Research Centre, Coventry University, Coventry CV1 5FB, England

Generalized-ensemble Monte Carlo simulations such as the multicanonical method and similar techniques are among the most efficient approaches for simulations of systems undergoing discontinuous phase transitions or with rugged free-energy landscapes. As Markov chain methods, they are inherently serial computationally. It was demonstrated recently, however, that a combination of independent simulations that communicate weight updates at variable intervals allows for the efficient utilization of parallel computational resources for multicanonical simulations. Implementing this approach for the many-thread architecture provided by current generations of graphics processing units (GPUs), we show how it can be efficiently employed with of the order of 10^4 parallel walkers and beyond, thus constituting a versatile tool for Monte Carlo simulations in the era of massively parallel computing. We provide the fully documented source code for the approach applied to the paradigmatic example of the two-dimensional Ising model as starting point and reference for practitioners in the field.

CPP 34.3 Tue 14:30 BH-N 128

Multiferroic properties of HoMn2O5 compounds: A Monte Carlo Study — •A.S ERCHIDI ELYACOUBI, R Masrour, and A Jabar — Cady Ayyed University, National School of Applied Sciences, PB 63 46000, Safi, Morocco.

The class of HoMn2O5 compounds offers multiferroic properties where the refined magnetic zig-zag order breaks the inversion symmetry. The polarization and magnetization are found. The ferroelectric transition temperature are determined. The polarization is induced solely by different exchange couplings of the two different Mn4+ and Mn3+ magnetic ions. The magnetic and ferroelectric cycle have been deduced. The variation of the polarization by an external magnetic field depends strongly on the direction of that field. HoMn2O5 compounds;

CPP 34.4 Tue 14:45 BH-N 128

Identifying the relevant degrees of freedom in mesoscale models of liquid water with Bayesian formalism — •Julija Zavadlav and Petros Koumoutsakos — Computational Science and Engineering Laboratory, ETH Zurich, Zurich, CH-8092, Switzerland

Coarse-graining (CG) has become an established methodology in molecular modeling to access time and length scales that are computationally beyond the reach of the conventional atomistic simulations. However, it often involves making several a priori assumptions, which are rarely systematically addressed. Typically, these assumptions pertain to the level of coarse-graining and the model complexity. We address this issue for mesoscale models of liquid water by investigating on an equal footing a number of CG models that differ in the level of coarse-graining and in the model complexity. To this end, we deploy the classical as well as a novel Hierarchical Bayesian methods [1,2] to quantify and calibrate the uncertainty of the models and to perform the model selection using the experimental data. Furthermore, we assess the efficiency-accuracy trade-off of developed models and provide guidelines for future water model design at the mesoscopic scale.

[1] S.Wu, P. Angelikopoulos, G. Tauriello, C. Papadimitriou, and P. Koumoutsakos, J. Chem. Phys. 145, 244112, 2016.

[2] L. Kulakova, G. Arampatzis, P. Angelikopoulos, P. Hadjidoukas, C. Papadimitriou, and P. Koumoutsakos, Sci. Rep., 7, 16576, 2017

CPP 34.5 Tue 15:00 BH-N 128

Data driven inference for the repulsive exponent of the Lennard-Jones potential in molecular dynamics simulations — •Georgios Arampatzis and Petros Koumoutsakos — Computational Science and Engineering Laboratory, Clausiusstrasse 33, ETH Zürich, CH-8092, Switzerland

The Lennard-Jones (LJ) potential is a cornerstone of Molecular Dynamics (MD) simulations and among the most widely used computational kernels in science. The LJ potential models atomistic attraction and repulsion with century old prescribed parameters ($q = 6$, $p = 12$, respectively), originally related by a factor of two for simplicity of calculations. We propose the inference of the repulsion exponent through Hierarchical Bayesian uncertainty quantification We use experimental data of the radial distribution function and dimer interaction energies from quantum mechanics simulations. We find that the repulsion exponent $p \approx 6.5$ provides an excellent fit for the experimental data of liquid argon, for a range of thermodynamic conditions, as well as for saturated argon vapour. Calibration using the quantum simulation data did not provide a good fit in these cases. However, values $p \approx 12.7$ obtained by dimer quantum simulations are preferred for the argon gas while lower values are promoted by experimental data. These results show that the proposed LJ 6-p potential applies to a wider range of thermodynamic conditions, than the classical LJ 6-12 potential. We suggest that calibration of the repulsive exponent in the LJ potential widens the range of applicability and accuracy of MD simulations.

CPP 35: Microswimmers I (joint session DY/BP/CPP)

Time: Tuesday 14:00–15:45 Location: BH-N 243

CPP 35.1 Tue 14:00 BH-N 243

Active colloidal propulsion over a crystalline surface — Udit Choudhury[1], •Arthur Straube[2], Peer Fischer[1], John Gibbs[3], and Felix Höfling[2] — [1]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany — [2]Freie Universität Berlin, Institute of Mathematics, Berlin, Germany — [3]Department of Physics and Astronomy, Northern Arizona University, Flagstaff, USA

We study both experimentally and theoretically the dynamics of chemically self-propelled Janus colloids moving atop a two-dimensional (2d) crystalline surface [1]. The surface is a hexagonal close-packed monolayer of colloidal particles of the same size as the mobile one. The dynamics of the self-propelled colloid reflects the competition between hindered diffusion due to the periodic surface and enhanced diffusion due to active motion, which can be tuned by changing the concentration of a chemical fuel. Our experimental data for the mean-square displacements (MSDs) are consistent with a Langevin model for the effectively 2d translational motion of an active Brownian particle in a periodic potential, combining the confining effects of gravity and the crystalline surface with the free rotational diffusion of the colloid. Approximate analytical predictions are made for the MSD describing the crossover from free Brownian motion at short times to active diffusion at long times. The results are in semi-quantitative agreement with numerical results of a refined Langevin model that treats translational and rotational degrees of freedom on the same footing.

[1] U. Choudhury, A. V. Straube, P. Fischer, J. G. Gibbs, F. Höfling, New J. Phys. (2017), doi: 10.1088/1367-2630/aa9b4b

CPP 35.2 Tue 14:15 BH-N 243

Dynamics of a single circular microswimmer in a quenched crowded media — •Oleksandr Chepizhko and Thomas Franosch — Institute for Theoretical Physics, University of Innsbruck, Innsbruck, Austria

The motion of active particles, for example, bacteria or unicellular organisms, in nature occurs in crowded environments such that the walls, boundaries, and obstacles strongly influence the dynamics of the microswimmers. Here we present a generic model for a deterministic circular microswimmer in a disordered two-dimensional quenched random array of obstacles. The microswimmer moves in circular orbits between the collisions with the obstacles, and after colliding with an obstacle the microswimmer follows the obstacle's surface for some time before detaching again.

The diffusivity of the system is studied via event-driven computer simulations for a wide range of obstacle densities and orbit radii. We find to phase boundaries of a conducting phase with an insulating and a localized phase. The phase behavior is investigated both close to these two transition lines, as well as deep in the conducting phase. The phase transitions correspond to critical phenomena with both an underlying static percolation transition, while the dynamic exponents reveal different universal classes. Furthermore, we find that the diffusivity grows with the density of obstacles up to a narrow region in the vicinity of the localization transition where it rapidly drops to zero.

CPP 35.3 Tue 14:30 BH-N 243

Controlled Control of Cargo Delivery Performed by Self-Propelled Janus Droplets — •Menglin Lee[1], Martin Brinkmann[1], Ignacio Pagonabarraga[2], Ralf Seemann[1], and Jean-Baptiste Fleury[1] — [1]Saarland University, Saarbruecken, Germany — [2]University of Barcelona, Bracelona, spain

We propose a class of programmable carrier droplets that can be made of a water/ethanol mixture dispensed in a continuous oil/surfactant solution. While swimming, the droplets pass through up to three stages whose appearance and duration are determined by the chemical composition of the droplet and the surrounding phase. A spontaneous de-mixing of the initially homogeneous droplet phase controlled by an uptake of surfactant and simultaneous loss of ethanol is generally observed. The phase segregation can lead to the formation of characteristic Janus droplets which consist of a water-rich and an ethanol-rich droplet. During de-mixing cargo molecules, like DNA, can be separated in the trailing ethanol–rich droplet and are "carried like in a backpack". Delivery is obtained whenever the trailing droplet touches a wettable target. Selective attraction or repulsion from targets is determined by the long–range hydrodynamic interactions of the swimmers with the geometric shape of the targets. In combination with a controlled delay of phase separation by the initial chemical composition of the droplets, we can exploit this selectivity to deliver DNA molecules dissolved in the ethanol-rich droplet at specific target sites and during a specific timeframe.

(under review - 2017)

CPP 35.4 Tue 14:45 BH-N 243

Clearing out a Maze: Chemotaxis and Percolation — Tanja Schilling[1] and •Thomas Voigtmann[2,3] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany — [2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [3]Department of Physics, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany

We study chemotactic motion in a random environment of obstacles by means of a lattice model that bears resemblance to the arcade game PAC-MAN®: A random walker moves on the percolating cluster of a square lattice, with steps that are biased towards the food that is initially placed on the accessible lattice sites and that is then consumed by the walker. Anomalous diffusion emerges, and is best described by a power-law with a non-trivial dynamical exponent that depends continuously on the propensity of the walker to move towards food. Although its food propensity biases the walker to explore previously unvisited sites more easily than the unbiased random walk, and thus intuitively serves to stretch out the walker's trajectories in comparison to the non-chemotactic case, the asymptotic growth of the mean-squared displacement is weaker. We suggest that getting lost in the culs-de-sac is a mechanism to explain why the chemotactic exploration of a maze thus becomes less effective than the pure diffusive one.

[1] T. Schilling and Th. Voigtmann, J. Chem. Phys. (in press, 2017); arXiv:1607.01123.

CPP 35.5 Tue 15:00 BH-N 243

Theoretical study of triangular magnetocapillary microswimmers — •Alexander Sukhov[1], Sebastian Ziegler[2], Oleg Trosman[2], Ana-Suncana Smith[2], and Jens Harting[1,3] — [1]Helmholtz Institute Erlangen-Nuernberg for Renewable Energy (IEK-11), Forschungszentrum Juelich GmbH, 90429 Nuernberg, Germany — [2]Institute for Theoretical Physics, Friedrich-Alexander University Erlangen-Nuernberg, 91054 Erlangen, Germany — [3]Department of Applied Physics, Eindhoven University of Technology, NL-5600MB Eindhoven, The Netherlands

As demonstrated experimentally (for a recent review see Ref. [1]), magnetocapillary swimmers - a system of three or more magnetic beads trapped at a fluid-gas interface - prefer to form equilateral triangles due to an interplay of attractive capillary and repulsive magnetic dipole-dipole interactions. By applying additionally a time-dependent magnetic field the position of the swimmer and its velocity direction can be wirelessly manipulated. Combining the lattice Boltzmann method with the analytical force-based bead-spring model [2, 3] extended for a triangular configuration, we explain a sharp dependence of the average speed of the swimmer on the frequency of the time-dependent magnetic field and compare our results with the experiment. In addition, we demonstrate numerically and analytically the control of the direction of the swimmer motion using magnetic fields. [1] G. Grosjean, M. Hubert and N. Vandewalle, Adv. Colloid Interface Sci., in press (2017); [2] B.U. Felderhof, Phys. Fluids **18**, 063101 (2006); [3] J. Pande *et al.*, New J. Phys. **19**, 053024 (2017).

CPP 35.6 Tue 15:15 BH-N 243

The frequency-dependent behavior of microswimmers in oscillating shear flow — Kevin Schröer[1], •Patrick Kurzeja[2], and Lothar Brendel[1] — [1]Faculty of Physics and CeNIDE, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Institue of Mechanics, Technical University Dortmund, 44227 Dortmund, Germany

One possibility to alter the macroscopic properties of a self-propelled nanoparticle suspension is the introduction of inhomogeneities in the propulsion mechanism, which leads to drastic changes in the collective behavior [1].

A new approach is presented for sheared suspensions: the control via oscillating walls. The oscillation frequency determines the thickness of a viscous boundary layer that surrounds the inertia-dominated center region. This is characterized by the Womersley number Wo, being the ratio between viscous and inertial forces [2]. As a result, regions of particle rotation and translation can be varied by this frequency.

Using this setup, we investigate the impact of Wo on the rheology of a dilute microswimmer suspension by means of Multi-Particle Collision Dynamics (MPC) simulations. This method is suited to capture hydrodynamics and thermal fluctuations and has been used in related topics like dilute suspensions in a gravity perturbed annular shear [3] or bidisperse segregation in a Hagen-Poiseuille flow [4].

[1] M. P. Magiera and L. Brendel, Phys. Rev. E 92, 1 (2015)
[2] P. Kurzeja et al., JASA 140, 4378 (2016)
[3] K. Schröer et al., EPJ Web of Conferences, 140 (2017)
[4] P. Kanehl and H. Stark, J. Chem. Phys. 142, 214901 (2015)

CPP 35.7 Tue 15:30 BH-N 243

Buckling instability and swimming of elastic spherical shells — •Adel Djellouli[1], Philippe Marmottant[1], Henda Djeridi[2], Catherine Quilliet[1], and Gwennou Coupier[1] — [1]Univ. Grenoble Alpes, CNRS, LIPhy, 38000 Grenoble, France — [2]Univ. Grenoble Alpes, Grenoble INP, CNRS, LEGI, 38000 Grenoble, France

Under pressure, a hollow elastic sphere becomes unstable and collapses. It reinflates back when the pressure is decreased. The shape hysteresis associated to this deformation cycle makes this simple object a good candidate for becoming a microswimmer, that is, a swimmer able to move at low Reynolds number.

We explore this possibility through a macroscopic experiment in fluids of varying viscosities so as to explore different flow regimes [1]. We show that not only the shape sequence hysteresis leads to swimming but the asymetry in the deformation velocity makes the fast buckling phase an efficient mechanism for propulsion that implies inertial effects and subtle coupling between shape post-buckling oscillations and fluid flow patterns. Our modeling shows that such an inertial regime could even be reached at microscopic scale.

We anticipate that a conveyor made of a few of microbubbles with different shell thicknesses, would constitute a microrobot whose 3D displacement can be remotely controlled by an echographic device - a relatively cheap and widely available tool in the hospitals.

[1] A. Djellouli, P. Marmottant, H. Djeridi, C. Quilliet and G. Coupier, Phys. Rev. Lett. 119, 224501 (2017). See also P. Ball, "Focus: Elastic Spherical Shell Can Swim", Physics 10, 128 (2017).

CPP 36: Particulate Matter: From microscopic interactions to collective motion (joint session DY/CPP)

Time: Tuesday 14:00–15:45 Location: EB 107

CPP 36.1 Tue 14:00 EB 107

Onset of anomalous diffusion in colloids confined to quasimonolayers — •Martin Oettel[1], Johannes Bleibel[1], and Alvaro Dominguez[2] — [1]Institut für Angewandte Physik, Universität Tübingen — [2]Fisica Teorica, Universidad de Sevilla

It has been recently shown that a colloidal monolayer, e.g., formed at a fluid interface or by means of a suitable confining potential, exhibits anomalous collective diffusion: diffusion becomes accelerated as signalled by a $1/k$–divergence of the wavenumber–dependent collective diffusion coefficient. This is a consequence of the hydrodynamic interactions mediated by the three-dimensional (3D) ambient fluid when the particles are confined to reside on a two-dimensional (2D) manifold. We study theoretically and with numerical simulations the crossover from normal to anomalous diffusion as the particles are, in real systems, confined by a 3D external potential and thus have the possibility to fluctuate out of the 2D manifold, thus forming a quasimonolayer. In essence, we always find anomalous diffusion on lateral length scales larger than the confinement width.

CPP 36.2 Tue 14:15 EB 107

Microrheology in hard colloids with large tracers — •Antonio M. Puertas[1], Francisco Orts[2], Gloria Ortega[2], and Ester M. Garzon[2] — [1]Dpt. of Applied Physics, Univ. of Almeria, Almeria, Spain — [2]Dept. of Informatics, Univ. of Almeria, Agrifood Campus of Int. Excell., ceiA3, Almeria, Spain

Microrheology has become recently in a powerful technique to study the dynamics of a system in microscopic scales. A colloidal tracer is introduced in the host system, and its dynamics is monitored. When an external force acts on the tracer, the system goes out of equilibrium probing the linear regime for small forces, and entering the non-linear regime for large ones. A colloidal bath of hard spheres is probably the simplest example. Several theory models have been developed, tested by simulations, but typically these restrict to tracers of the same size as the bath particles.

Here, we present simulation results of the dynamics of a tracer pulled with a constant force in a colloidal bath. The tracer size, a_t, is larger than the bath particles, size a, up to $a_t = 5a$. Important finite size effects appear, particularly for large tracers, which have been studied and compared with predictions from hydrodynamics for the bath. Due to the massive computational demand, the simulations were computed on a multiGPU cluster and a genetic algorithm was designed to optimize the performance. The dynamics of the tracer, providing the friction coefficient with the bath and the effects of the bath (density fluctuations, and strain field) are studied for small forces. The theoretical limit of an infinite tracer, $a/a_t \to 0$, and small forces, is checked.

CPP 36.3 Tue 14:30 EB 107

Efficient simulation of anisotropic particles using collective Monte Carlo moves — •Marco Klement and Michael Engel — Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Hard anisotropic particles are a classical model for the influence of shape on the thermodynamic behaviour of particulate matter. Examples are the phase diagram of liquid crystal formers and the prediction of crystal structures for polyhedral nanocrystals [1]. Here, we investigate the speed-up of hard polyhedra Monte Carlo simulations by using collective chain moves [2]. Our implementation relies on analytically detecting sweep collisions with an improved version of the Minkowski portal refinement algorithm. We validate our method by calculating equations of state and studying self-assembly phenomena.

[1] M.A. Boles, M. Engel, D.V. Talapin, Chem. Rev. 116, 11220-11289 (2016).

[2] E.P. Bernard, W. Krauth, D.B. Wilson, Phys. Rev. E 80, 056704 (2009).

CPP 36.4 Tue 14:45 EB 107

Stochastic Nature of Granular Tribocharging — •Jan Haeberle[1], André Schella[2], Matthias Schröter[2], Matthias Sperl[1], and Philip Born[1] — [1]Deutsches Zentrum für Luft- und Raumfahrt, Köln, Deutschland — [2]MPI Dynamics and Self-Organization, Göttingen, Germany

Triboelectric charging of granular media has important consequences for the bulk behaviour. Effects such as powder flowability or cluster formation due to charging are everyday experiences [1]. Triboelectric charging has also been linked to segregation [2] and suggested as a tool for structure formation in granular media [2,3]. Recently, the stochastic nature of the triboelectric charging process has become apparent [4]. To further investigate the stochastics of tribocharging, we have studied the distribution resulting after a tribocharging event in a custom-made Faraday cup setup. We measure non-Gaussian asymmetric charge distributions. We find, that we can describe the measured distributions by a model combining a distinct stochastic charging and stochastic discharging process.

[1] Duran, J., Sands, Powders, and Grains, Springer, New York (2000) [2] Schella, A., Herminghaus, S. & Schröter, M., Soft Matter 13, 394-401 (2017). [3] Cademartiri, R. et al., Soft Matter 8, 9771 (2012). [4] Apodaca, M. M., Wesson, P. J., Bishop, K. J. M., Ratner, M. A. & Grzybowski, B. A., Angewandte Chemie 122, 958-961 (2010).

CPP 36.5 Tue 15:00 EB 107

Universal hidden order in amorphous cellular geometries — •Michael A. Klatt[1], Jakov Lovrić[2,3], Duyu Chen[4], Sebastian C. Kapfer[5], Fabian M. Schaller[5,1], Philipp W. A.

Schönhöfer[3,5], Bruce S. Gardiner[3], Ana-Sunčana Smith[2,5], Salvatore Torquato[4,6], and Gerd E. Schröder-Turk[3,5] — [1]KIT, Institute of Stochastics, 76049 Karlsruhe, Germany — [2]Division of Physical Chemistry, Ruder Bošković Institute, Zagreb, Croatia — [3]Murdoch University, School of Engineering and Information Technology, 90 South St, Murdoch WA 6150, Australia — [4]Department of Chemistry, Princeton University, New Jersey 08544, USA — [5]Institute for Theoretical Physics, FAU, 91058 Erlangen, Germany — [6]Department of Physics, PRISM, PACM, Princeton University, New Jersey 08544, USA

Starting from an amorphous partitioning of space into cells, we iteratively optimize the “centrality” of the cells, minimizing the so-called Quantizer energy. The energy landscape is replete with local minima to which the system converges despite the existence of lower-energy crystalline configurations. Irrespective of the level and type of disorder in the initial configurations, the tessellations converge to the same amorphous state, as measured by the same structure factor and energy distributions. The final disordered configurations exhibit an anomalous suppression of long-wavelength density fluctuations, known as hyperuniformity. For systems related to the Quantizer problem, such as self-assembled copolymeric phases, our findings suggest the possibility of stable disordered hyperuniform phases.

CPP 36.6 Tue 15:15 EB 107

Relaxation of hydrogen bond network in water subject to E-field — •Andreas Baer[1], Zoran Milicevic[1,2], David Matthew Smith[2,3], and Ana-Suncana Smith[1,2] — [1]PULS Group at the Institute for Theoretical Physics and EAM, FAU Erlangen-Nürnberg, Germany — [2]Division of Physical Chemistry, Institute Ruđer Bošcović, Zagreb, Croatia — [3]Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

Most of the amazing properties of liquid water stem from the fluctuations in the uninterrupted network of hydrogen-bonded molecules.[1] One such phenomena is the splitting of transport coefficients in an electric field, which despite the enormous technological implication, is an effect not yet understood from the microscopic point of view. We address this problem by simulating pure water in a uniaxial E-field under ambient conditions using the GROMACS framework.[2] After quantifying the translational and orientational dynamics of water molecules, characteristic, anisotropic timescales for the reordering of hydrogen bonds are retrieved. A novel relaxation process occurring on the picosecond timescale is detected, and unambiguously associated with cooperative rotations of multiple hydrogen-bonded molecules that induce a slow relaxation of components of the macroscopic shear viscosity that are parallel to the field direction.[3] [1] Luzar, A.; Chandler, D. Nature 1996 379, 55-57. [2] Milicevic Z., Marrink S. J., Smith A.-S., Smith D. M. J. Mol Mod 2014 20, 2359 [3] Milicevic Z., Baer A., Smith D. M., Smith A.-S., PRX submitted

CPP 36.7 Tue 15:30 EB 107

In-cage dynamics of molecular hydrogen in clathrates hydrates as function of the confinement size — •Margarita Russina — Helmholtz Zentrum Berlin für Materialied und Energie, Hahn-Meitner Platz 1, 14109 Berlin

To understanding the criteria governing the molecular mobility in confinement we have studied in-cage dynamics of confined molecular hydrogen as a function of confinement size. We used nanopores ice based clathrate with nanocages of two different dimensions of 0.75 and 0.946 nm, which are particularly suitable model systems since the interactions between the clathrate framework and H2 are of the same hydrophobic nature in both cages. We have found that by varying the size of the pore by only 20 % in the effective radius we can modify the diffusive mobility of confined hydrogen in both directions, i.e. both reducing and enhancing mobility compared to the bulk. In the smaller cages of clathrate hydrates with a mean size of 0.795 nm we observe strong hydrogen localization in the cage center even at temperatures up to 200K. Moderate increase of the confinement to 0.946 nm leads to the onset of jump diffusion between tetrahedrally shaped sorption sites in large cages with separation length of about 2.79 Å already at T=10 K, where bulk hydrogen is frozen at ambient pressure. The observed difference in mobility between small and large cages can be understood as a dimensional phenomenon caused by the modulation of cage potentials as a function of the cage size.

CPP 37: Focus: Smart Hydrogels and Hydrogel Based Devices II - organized by Gerald Gerlach, Walter Richtering and Thomas Hellweg

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

Topical Talk CPP 37.1 Wed 9:30 C 130

Enzyme-functionalized polymer microgels for drug building block synthesis — •Julian Thiele — Leibniz-Institut für Polymerforschung Dresden e.V. / Leibniz Research Cluster, Dresden, Germany

In an attempt to close the current innovation gap in antibiotics research, we utilize highly specific, genetically engineered enzymes for drug synthesis in cell-free biotechnology. These enzymes require tailored experimental platforms that maintain enzyme activity, enhance the enzyme*s shelf life, and allow for extraction of valuable enzymes from reaction mixtures for recycling purposes. Being part of the Leibniz Research Cluster - an interdisciplinary network of five young investigator groups - we perform enzymatic reactions in polymer microgels with tailored size, porosity and functionalization. As material basis, we employ hyaluronic acid, which is cross-linked by mild [4+2]cycloaddition or thiol-Michael addition, and functionalized with Ni-NTA linker molecules to capture His-tagged enzymes. By loading these microgels into microreactors with active components (e.g. heating pads and valves), we tailor reaction conditions down to the micrometer scale and extract samples for in situ analytics by HPLC-MS and CARS as well as colorimetric assays, which are designed towards individual reaction intermediates and products. We show the capability of this approach using the example of malonate-to-Malonyl CoA conversion, which is a key intermediate in the synthesis of polyketide-based drugs.

CPP 37.2 Wed 10:00 C 130

Vapor-deposited Thin Hydrogel Coatings for Controlled Drug Release — Stephan Tumphart[1,2], •Paul Christian[1], Anna Coclite[1], and Oliver Werzer[2] — [1]Inst. f. Solid State Physics, Graz University of Technology, Austria — [2]Pharm. Tech. & Biopharmacy, University of Graz, Austria

Polymers can have a wide range of applications in the field of pharmaceutical formulation but are most often employed for controlled release behavior. ”Smart polymers”, meaning polymers that change chemical and physical properties depending on the environment they are in, are particularly interesting as they allow for a targeted release. However, the preparation of thin & defined polymer coatings atop of drug layers is usually difficult by common solution techniques. Initiated Chemical Vapor Deposition (iCVD), a solvent-free polymerization technique, is a powerful tool to conformally prepare thin polymer layers even on delicate substrates. In this study, the release behavior of model pharmaceuticals such as Indomethacin and Clotrimazole is investigated when coated either with a hydrogel or with a thermally-responsive polymer (NIPAAm). Depending on mesh size, polymer and temperature, the release behavior could be varied between several orders of magnitude.

CPP 37.3 Wed 10:15 C 130

Mechano-responsive Coiled Coil-based Hydrogels as Extracellular Matrix Mimics — •Alberto Sanz de Leon, Melis Goktas, Patricia Lopez Garcia, and Kerstin Blank — Max Planck Institute of Colloids and Interfaces, Mechano(bio)chemistry, Potsdam-Golm Science Park, 14424 Potsdam, Germany

Coiled coils (CCs) are protein motifs consisting of at least two α-helices wound into a superhelix. Besides providing structural support, CCs are also involved in different biomechanical signaling processes as they possess a well-defined response to mechanical loads. Considering their natural function as mechano-responsive building blocks, we have synthesized biomimetic hydrogels, using different CC sequences as dynamic, reversible crosslinks. These hydrogels can be fully disassembled and reassembled, showing well-defined self-healing properties. Observing their frequency-dependent behavior at different temperatures and strain rates, we are able to quantify thermodynamic and mechanical processes within these hydrogels. Their bulk mechanical response is well described by the Maxwell model for viscoelastic liquids. Using the Bell-Evans model, we are able to extract molecular parameters that describe CC rupture in the hydrogels. Comparing with single molecule force spectroscopy experiments, we show that this approach is sufficiently accurate to quantitatively extract molecular information from bulk viscoelastic parameters. These results lay the foundation for the future application of these hydrogels as smart mechano-responsive ECM mimics for dissecting local and global factors that determine the process of cellular mechanosensing.

CPP 37.4 Wed 10:30 C 130

Gene expression in NTA-hyaluronan hydrogel particles: A strategy for in situ separation and purification of His-tagged proteins — •THOMAS HEIDA, TONY KÖHLER, ANDREAS FERY, and JULIAN THIELE — Leibniz Institut für Polymerforschung e.V., Dresden, Germany

We present the synthesis and characterization of nitrilotriacetic acid (NTA)-modified hydrogel particles as well as their application in in vitro transcription/translation (IVTT), to selectively catch and separate expressed proteins in situ. Droplet microfluidics is employed to fabricate hydrogel particles based on furan-functionalized hyaluronic acid and maleimide-modified poly(ethylene glycol) (PEG) crosslinkers. As a proof of principle, we show selective conjugation and release of His-tagged green fluorescent protein (GFP) within the particles by reversible binding via Ni(II)-complexation. Thereafter, we utilize these particles as experimental platform in in vitro transcription/translation (IVTT) by additional functionalization with DNA encoding for His-GFP. In situ formed proteins are selectively separated from the complex IVTT reaction mixture and controllably released from the gel matrix after purification. Our NTA-hyaluronan microgels serve as robust experimental platform for cell-free synthesis and purification of His-tagged proteins.

15 min. break

Topical Talk CPP 37.5 Wed 11:00 C 130

Microgel-functionalized membranes — •Matthias Wessling — DWI Leibniz Institute for Interactive Materials, Aachen, Germany

Microgels are interactive soft colloids that can be triggered and tuned. They change size, charge, and density. This presentation explores the use of microgels to functionalize synthetic membranes. Examples will demonstrate that (a) temperature modulation tunes size exclusion (b) charge control influences electro-static repulsion of charged organic dye molecules while passing uncharged molecules of an even larger size (c) monolayers of microgels tune the monovalent/bivalent ion selectivity of synthetic ion exchange membranes (d) printed dotlike patterns of microgel monolayers effectively actuate chaotic electro-convection at polarized ion exchange membrane.

CPP 37.6 Wed 11:30 C 130

Smart membranes by electron beam cross-linking of copolymer microgels — •Johannes Bookhold and Thomas Hellweg — Universität Bielefeld, Bielefeld, Deutschland

The aim of this contribution is the preparation of free-standing, transferable microgel layers from cross-linkable microgels. The approach is based on the deposition of microgels, containing aromatic moieties, by spincoating on a sacrificial gold layer. During this work NIPAm has been copolymerized with N-Benzylhydrylacrylamide (BHAm) in order to manufacture novel cross-linkable microgels. After confirmation of the incorporation of the copolymer via PCS and IR-spectroscopy measurements into the polymer network, monolayers of the microgels were spin-coated onto gold coated silicon-wafers. Afterwards the incorporated aromatic comonomers were irradiated using an electron beam leading to a cross-linking of the microgels. The cross-linked microgel-monolayer was detached from the wafer through the dissolving of the gold coating in an acidic environment. In order to perform temperature dependent diffusion measurements the detached membrane was transferred onto a silica-nitrate chip with a pinhole. In a microfluidic device the diffusion through the covered pinhole was determined using conductivity measurements.

CPP 37.7 Wed 11:45 C 130

Influence of the surface confinement on the structural properties of adsorbed microgel particles — •Tetyana Kyrey[1,2], Judith Witte[1], Regine von Klitzing[3], Stefan Wellert[1], and Olaf Holderer[2] — [1]Technische Universität Berlin, Berlin, Germany — [2]JCNS at MLZ, Garching, Germany — [3]Technische Universität Darmstadt, Darmstadt, Germany

In the last few decades a lot of work was devoted to investigate stimuli-responsive *smart* polymer systems. The main feature of such systems is their ability to rapidly react to an external stimulus such as temperature, light or solvent quality. Of special interest are stimuli responsive polymer systems at interfaces. Due to surface confinement their ability to dramatically change the characteristic sizes is limited. In the current work, the structural properties of adsorbed individual poly(N-isopropylacrylamide)(PNIPAM) microgel particles on Si-blocks by means of AFM, neutron reflectometry and grazing incidence small-angle neutron scattering (GISANS) are investigated. We discuss PNIPAM microgel particles in dependence on the crosslinker content (N,N-methylenebisacrylamide, 0.5 and 5%) at temperatures below and above the volume phase transition temperature (VPTT). The influence of the surface confinement on the swelling process and possibility to form individual particles on the surface at the different crosslinker content are presented.

CPP 37.8 Wed 12:00 C 130

Hydrogels for Microsensors - Mechanical Properties and Swelling Forces of Microgel Particles — •Maximilian Seuss[1], Willi Schmolke[2], Sebastian Seiffert[2], Astrid Drechsler[1], Ivan Raguzin[1], Julian Thiele[1], and Andreas Fery[1] — [1]Leibniz Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Institute of Physical Chemistry, Johannes Gutenberg-Universität, Mainz, Germany

Hydrogels have drawn the focus of engineers to be applied in microsensors since many hydrogels exhibit a volume phase transition reacting to an external stimulus, e.g. changes in the pH, temperature or concentration of specific molecules. Here we present an approach for core-shell microgel particles which are responsive to temperature while the surface adhesion stays unaltered. This is achieved by encapsulating a pre-prepared poly(N-isopropylacrylamide) (pNiPAAm) microgel particle with a poly(acrylamide) shell in a microfluidic reactor. Combining optical microscopy and colloidal probe AFM measurements we demonstrate that the responsiveness as well as the accompanied changes in mechanical properties can be detected on the per-se unresponsive shell.[1] Furthermore, the colloidal probe technique is applied to directly measure the exerted swelling force of single confined model pNiPAAm hydrogel particle. Combining the network architecture with the changes in volume, mechanical compliance and resulting swelling forces may provide important parameters for novel sensor designs.

[1] M. Seuss, W. Schmolke, A. Drechsler, A. Fery, S. Seiffert, ASC Appl. Mater. Interfaces, 2016, 8, 16317

CPP 37.9 Wed 12:15 C 130

Properties and internal structure of thermoresponsive acrylamide based core-shell microgels — •Marian Cors[1,2], Oliver Wrede[1], Julian Oberdisse[2], and Thomas Hellweg[1] — [1]Bielefeld University, Bielefeld, Germany — [2]Laboratoire Charles Coulomb, Université de Montpellier, Montpellier, France

A gel is a dispersed system which consists of at least two different components: a solid or flexible mesh and a fluid (water in the present case). Microgels are gels in the size range of 10 nm to 1 μm and can be used in a wide range of applications like drug delivery and smart surface coatings. If the microgel consists of acrylamides like N-isopropylmethacrylamide (NIPMAM) or N-n-propylacrylamid (NNPAM) as network component, they show a volume phase transition (VPT) at a certain temperature, the volume phase transition temperature (VPTT). An increase in temperature above the VPTT leads to an abrupt decrease in size and a decrease in temperature leads to an abrupt increase in size. The VPTT is specific for each monomer. To use microgels in sensors or for nanoactuators the thermoresponse has to be precise. That is why we investigated microgels with a core-shell architecture containing NIPMAM and NNPAM. These particles show a tunable linear change in size between 22 °C and 43 °C. Furthermore, we deposited these microgels on surfaces and investigated the properties of the coating. The properties of these particles and coatings can be adjusted by selecting specific synthesis conditions. We then did small angle neutron scattering (SANS) to determine the internal structure of the core-shell microgel.

CPP 37.10 Wed 12:30 C 130

Feringa Type Engines in Polymer Model Systems: Folding, Coiling, Molecular Stirling Engines, and Active Gels — •Cornelia Schuster[1,2], Michael Lang[1], Ron Dockhorn[1,2], Martin Wengenmayr[1,2], and Jens-Uwe Sommer[1,2] — [1]Institut Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Straße 6, 01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, Zellescher Weg 17, 01069 Dresden, Germany

We use the bond fluctuation model to study the contraction process of different polymeric model systems with attached Feringa engines, where the top part of the molecule rotates unidirectional with respect to the bottom part upon irradition with light. For a figure of 8 shaped model system, a contraction process is observed that consists of two steps: folding followed by coiling. Double stranded polymers are studied in a slit geometry where either both strands connected to bottom and top of engine are connected to the bottom and top wall respectively (X geometry) or always only one strand connects to a particular wall (H-geometry). The different attachment causes distinct work cycles that allows to consider a Stirling machine that is either efficient at a small (H-geometry) or at a large wall separation (X-geometry). Insertion of the engines as centers of 4-functional stars in star polymer nano-gels leads to gel shrinkage upon irradiation with light as a function of the quantity of adsorbed light. The results of the first two model systems are used to elucidate the effectiveness of the engines inside the gel.

CPP 37.11 Wed 12:45 C 130

Silo outflow of soft frictionless hydrogel spheres — •Ahmed Ashour[1], Torsten Trittel[1], Tamás Börzsönyi[2], and Ralf Stannarius[1] — [1]Institute of Experimental Physics, Otto von Guericke University, Magdeburg, Germany — [2]Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Hungarian Academy of Sciences, Budapest, Hungary

The outflow of hard grains with different shapes and types in 2D and 3D silos has been extensively studied. The availability of incompressible but deformable hydrogels in recent years opened the door to study the effects of softness and nearly zero friction on the outflow of grains from silos with small aperture under the influence of gravity. We conduct a quasi-2D silo experiment with hydrogel spheres. This material shows new qualitative and quantitative features as compared to hard grains: The silo does not clog even when the orifice size is only slightly larger than two spheres in diameter. By decreasing the orifice size below two sphere diameters, intermittency of the flow rapidly increases, followed by a permanently clogged state. The soft spheres clog at a certain container fill height, unlike hard grains which flow out practically independent of the container fill level. The Janssen effect, a saturation of the pressure in a silo with fill height, is obviously ineffective for the soft frictionless material, the pressure at the silo bottom increases linearly with fill height (hydrostatic). On the other hand Beverloo's equation that describes the mass flow rate remains valid. Another important difference to hard grain silo discharge is that above a certain height respective to the orifice, the spheres above move in plug flow.

CPP 38: Modeling and Simulation of Soft Matter II (joint session CPP/DY)

Time: Wednesday 9:30–12:00 Location: C 230

Invited Talk CPP 38.1 Wed 9:30 C 230

The favorite polymer libations — •Carlos M. Marques[1], Debashish Mukherji[2], and Kurt Kremer[2] — [1]Institut Charles Sadron, UdS-CNRS, Strasbourg, France — [2]Max-Planck Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz Germany

Macromolecular solubility in solvent mixtures often strikes as a paradoxical phenomenon. In a system where all particle interactions are repulsive, chains can nevertheless collapse. And when attractive interactions settle in, they might collapse or swell the chain. We will review in this contribution how the puzzling behavior of polymers in aqueous alcohol solutions triggered a better understanding of the interplay between solvent composition and polymer conformation. And how the resulting view on polymer collapse and swelling takes us well beyond mean-field descriptions ... and alcohol.

[1] Mukherji, D., Marques, C. M., Kremer, K. (2014). Polymer collapse in miscible good solvents is a generic phenomenon driven by preferential adsorption. Nature communications, 5882, 5.

[2] Mukherji, D., Marques, C. M., Stuehn, T., Kremer, K. (2015). Co-non-solvency: Mean-field polymer theory does not describe polymer collapse transition in a mixture of two competing good solvents. The Journal of chemical physics, 142(11), 114903.

[3] Mukherji, D., Wagner, M., Watson, M. D., Winzen, S., de Oliveira, T. E., Marques, C. M., & Kremer, K. (2016). Relating side chain organization of PNIPAm with its conformation in aqueous methanol. Soft Matter, 12(38), 7995.

[4] Mukherji, D., Marques, C. M., Stuehn, T., Kremer, K. (2017). Depleted depletion drives polymer swelling in poor solvent mixtures. Nature communications, 1374, 8.

[5] Mukherji, D., Marques, C. M., Kremer, K. (2017). Collapse in two good solvents, swelling in two poor solvents: defying the laws of polymer solubility? Journal of condensed matter, 024002, 30.

CPP 38.2 Wed 10:00 C 230

Studying Polymer-induced Depletion Effects via Grid-based Simulations — •Qiyun Tang and Marcus Müller — Universität Göttingen, Institute für Theoretische Physik, Friedrich-Hund- Platz 1, 37077 Göttingen, Germany

Recently we found that our modified grid-based coarse-grained simulations could be employed to study the polymer induced depletion effects between nanoparticles in the nanoparticle/protein limit. By analysing the radial distribution function of nanoparticles from simulations, we systematically study the influence of polymer density and also the nanoparticle density on these depletion effects. Results show that in the semidilute region of polymer solution, the contact depletion potential is gradually reduced by increasing nanoparticle's concentration. Similar behavior is also observed in the polymer melt. The simulation results are also compared to the theories, and are consistent with the theoretical prediction in the dilute polymer solutions.

CPP 38.3 Wed 10:15 C 230

Process-directed assembly of copolymer materials — •Marcus Müller — Georg-August-Universität Göttingen, Institut für Theoretische Physik, Göttingen, Germany

Process-directed self-assembly of block copolymers refers to rapid thermodynamic processes that reproducibly direct the kinetics of structure formation from a starting, unstable state into a selected, metastable mesostructure. We investigate the kinetics of self-assembly of linear block copolymers after different rapid changes of thermodynamic control parameters (e.g., photochemical transformations, stretching or mechanical deformation, or pressure changes). These thermodynamic processes convert an initial, equilibrium mesophase of the copolymer material into a well-defined but unstable, starting state. The spontaneous structure formation that ensues from this unstable state becomes trapped in a metastable mesostructure, and we systematically explore, which metastable mesostructures can be fabricated by varying the physical properties of the copolymers in the starting and final state and a step-shear deformation. In addition to the equilibrium mesophases of linear AB diblock copolymers, this diagram of process-accessible states includes multiple, novel, metastable periodic mesostructures; inter alia, Schoen's F-RD periodic minimal surface. Strategies and challenges for studying process-directed self- assembly by particle-based simulations and self-consistent field theory are discussed and the role of non-equilibrium chain conformations and the diffusive dynamics is highlighted.

CPP 38.4 Wed 10:30 C 230

Non-covalent interactions across organic and biological subsets of chemical space: Physics-based potentials parametrized from machine learning — •Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Classical intermolecular potentials typically require an extensive parametrization procedure for any new compound considered. To do away with prior parametrization, we propose a combination of physics-based potentials with machine learning (ML), which is transferable across small neutral organic and biologically-relevant molecules. ML models provide on-the-fly predictions for environment-dependent local atomic properties across conformations and chemical compositions of H, C, N, and O atoms. These parameters enable accurate calculations of intermolecular contributions. Unlike other potentials, this model is transferable in its ability to handle new molecules and conformations without explicit prior parametrization: All local atomic properties are predicted from ML, leaving only eight global parameters—optimized once and for all across compounds. We validate IPML on various gas-phase dimers at and away from equilibrium separation, where we obtain mean absolute errors between 0.4 and 0.7 kcal/mol for several chemically and conformationally diverse datasets representative of non-covalent interactions in biologically-relevant molecules. We further focus on hydrogen-bond complexes—essential but challenging due to their directional nature—where datasets of DNA base pairs and amino acids yield an extremely encouraging 1.4 kcal/mol error.

15 min. break

CPP 38.5 Wed 11:00 C 230

Investigating structural and thermodynamic representability for coarse-grained models of ionic liquids — •Svenja Wörner[1], Joseph Rudzinski[1], Tamisra Pal[2], Michael Vogel[2], Kurt Kremer[1], and Tristan Bereau[1] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany. — [2]Technische Universität Darmstadt, Darmstadt, Germany.

Coarse-grained models are usually parameterized to reproduce either structure or thermodynamic properties. The coarse-grained model for the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate developed by Bhargava et al was parameterized to reproduce density and surface tension and therefore lacks detailed structural accuracy. In this work, we investigate to what extent the structural accuracy of this model can be improved while retaining the original thermodynamic target properties. We employ the generalized Yvon-Born-Green framework, which utilizes an integral equation theory that systematically connects the coarse-grained model parameters to the pair correlation functions. This methodology is not only useful for parameterizing new force fields , but can also be used to systematically perturb parts of potentials or to incorporate information from other state points to refine an existing force field. We demonstrate that perturbing only the hard core of the potential of the non-bonded interactions for ionic liquid model significantly improves the structure while retaining thermodynamic information included in the original model. Adding information from multiple temperatures may further improve representablility.

CPP 38.6 Wed 11:15 C 230

Mapping onto ideal chains profoundly overestimates self-entanglements in polymer melts — •Hendrik Meyer[1], Eric Horwath[2], and Peter Virnau[2] — [1]Institut Charles Sadron, CNRS and Université de Strasbourg — [2]Institut f. Physik, Universität Mainz

In polymer physics it is typically assumed that excluded volume interactions are effectively screened in polymer melts. Hence, chains could be described by an effective random walk. In this letter, we show that this mapping is problematic by analyzing the occurrence of knots, their spectrum and sizes in polymer melts, corresponding random walks and chains in dilute solution. The effective random walk severely overrates the occurrence of knots and their complexity, particularly when compared to melts of flexible chains, indicating that non-trivial effects due to remnants of self-avoidance still play a significant role for the chain lengths considered in this numerical study. For melts of semiflexible chains, the effect is less pronounced. In addition, we find that chains in a melt are very similar in structure and topology to dilute single chains close to the collapse transition, which indicates that the latter are also not well-represented by random walks. We finally show that typical equilibration procedures are well-suited to relax the topology in melts. [1] arXiv:1710.11077

CPP 38.7 Wed 11:30 C 230

Collective dynamics in liquid water: Molecular dynamics simulations — •Ari Paavo Seitsonen[1] and Taras Bryk[2] — [1]Département de Chimie, Ecole Normale Supérieure, Paris — [2]Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv

Water, as the most important substance for life, has always attracted the researchers to explore and explain its numerous anomalous properties. Collective dynamics in simple and molecular liquids is so far well understood only on macroscopic length and time scales. Experiments on Brillouin scattering of light on liquids can be described by the hydrodynamic theory, which explains the main relaxation and propagation processes contributing to the scattered intensity of light. Atomistic molecular dynamics simulations is an efficient tool in exploration of the dynamic properties, providing precious information on time-dependent correlations in liquids on nano- and atomic-scale resolution.

Here we report molecular dynamics simulations using density functional theory (DFT), in particular the BLYP approximation to the exchange-correlation term with the augmented D3 empirical term to account for the London dispersion interactions missing in the BLYP. We present results on the collective dynamics [1], and the recently evaluated [2] melting temperature of water using this approach.

[1] Taras Bryk & Ari P Seitsonen Condensed Matter Physics 19 (2016) 23604; DOI: 10.5488/CMP.19.23604

[2] Ari P Seitsonen & Taras Bryk Physical Review B 94 (2016) 184111; DOI: 10.1103/PhysRevB.94.184111

CPP 38.8 Wed 11:45 C 230

Molecular Origin of Urea-driven Hydrophobic Collapse of Polyacrylamides — •Divya Nayar, Angelina Folberth, and Nico van der Vegt — Technische Universität Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt, Germany

Osmolytes modulate protein folding and affect the water solubility of macromolecules [1]. The osmolyte-induced hydrophobic polymer collapse due to osmolyte depletion from the solvation shell is well-known, however, evidences have indicated direct preferential osmolyte binding that may lead to polymer collapse [2]. To understand the underlying molecular mechanisms better, we examine the role of urea in strengthening and attenuating the hydrophobic collapse of thermo-responsive polyacrylamides i.e. Poly-N-isopropylacrylamide (PNIPAM, secondary amide) and Poly-N,N,-diethylacrylamide (PDEA, tertiary amide) respectively [3]. Using extensive molecular dynamics simulations and large-scale polymer conformational sampling, we show that urea collapses PNIPAM by "preferentially binding" to it. We propose an osmolyte stabilizing mechanism driving PNIPAM collapse, based on the balance in opposing loss of entropic degrees of freedom of urea and water [4]. The study provides new physical insights into the interplay between polymer side-chain chemistry, solvent entropic degrees of freedom and polymer-solvent interactions to understand the osmolyte effects on hydrophobic collapse. [1] D. R. Canchi et al. Annu. Rev. Phys. Chem., 2013, 64, 273. [2] N. F. A. van der Vegt et al. J. Phys. Chem. B 2017, 121, 9986. [3] J. Wang et al. Macromolecules, 2016, 49, 234. [4] D. Nayar et al. Phys. Chem. Chem. Phys. 2017, 19, 18156.

CPP 39: Organic Photovoltaics II

Time: Wednesday 9:30–10:45 Location: C 243

Invited Talk CPP 39.1 Wed 9:30 C 243

Charge generation and recombination in an organic BHJ solar cell with low energetic offsets — •Thuc-Quyen Nguyen — Department of Chemistry and Biochemistry, University of California, Santa Barbara

Organic bulk heterojunction (BHJ) solar cells require energetic offsets between the donor and acceptor to obtain high short-circuit currents and fill factors. However, it is necessary to reduce the energetic offsets to achieve high open-circuit voltages. Recently, reports have highlighted BHJ blends that are pushing at the accepted limits of energetic offsets necessary for high efficiency. How the energetic offset impacts the solar cell characteristics thus remains poorly understood. We attempt to characterize the losses in BHJ blends that achieves a high open-circuit voltages with very low energy losses from the energy of absorbed photons. Despite the low energetic offset, the system does not suffer from field dependent generation and instead it is characterized by very fast nongeminate recombination and the presence of shallow traps. The charge-carrier losses are attributed to suboptimal morphology due to high miscibility between a polymer donor and PC61 BM. These results hold promise that given the appropriate morphology, the device parameters such as short-circuit currents, open-circuit voltages and fill factors can all be improved, even with very low energetic offsets.

CPP 39.2 Wed 10:00 C 243

A Shockley-type polymer:fullerene solar cell — •Safa Shoaee[1], Ardalan Armin[2], Zhiming Chen[3], Yaocheng Jin[3], Kai Zhang[3], and Fei Huang[3] — [1]Optoelectronics of Organic Semiconductors, Institute for Physics and Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany — [2]Centre for Engineered Quantum Systems, School of Mathematics and Physics, The University of Queensland, St Lucia Campus, Brisbane 4072, Australia — [3]Institute of Polymer Optoelectronic Materials and Devices, State Key Laboratory of Luminescent Materials and Devices, South China University of Technology, Guangzhou 510640, P. R. China.

Despite the myriad of organic donor:acceptor materials, only few systems have emerged in the life of organic solar cells to exhibit considerable reduced bimolecular recombination. Charge extraction rate in such devices is typically slow due to their low charge carrier mobility. Herein, we investigate charge transport and recombination properties of a ~10% efficient polymer (NT812):fullerene blend which delivers ~9% power conversion efficiency even when the junction thickness is as large as 800 nm. Experimental results indicate that this material system exhibits exceptionally low bimolecular recombination constant, 800 times smaller than the diffusion-controlled electron and hole encounter rate with nearly ideal charge collection. This is the first realization of high efficiency Shockley-type organic solar cells with junction thicknesses suitable for scaling-up.

CPP 39.3 Wed 10:15 C 243

Does electron delocalization influence charge separation at donor- — •Anna Köhler[1], Frank-Julian Kahle[1], Christina Saller[1], Selina Olthof[2], Cheng Li[1], Eva Herzig[1,3], and Peter Strohriegl[1] — [1]Universität Bayreuth, Bayreuth, Germany — [2]Universität Köln, Köln, Germany — [3]TUM, München, Germany

Recent reports on organic solar cells have shown that efficiencies of up to 13% are possible using a polymeric donor and a small molecular acceptor. Yet, fundamental processes governing efficient dissociation, especially at the donor-acceptor interface are still not fully understood. In this work, we use bilayer devices with a series of three fullerene acceptors differing in order, intermolecular coupling and LUMO localization to systematically explore the influence of electron delocalization in the acceptor phase on the dissociation efficiency of charge transfer states. Structural information from GIWAXS measurements are combined with the results of optical and electrical characterization via photocurrent and photoemission spectroscopy, electroabsorption and electroluminescence as well as theoretical modelling. We find that stronger intermolecular coupling and higher order within the acceptor phase is correlated with lower CT binding energies implying a higher degree of electron delocalization. Theoretical modelling of experimental field dependent photocurrent measurements reveals that an enhancement in electron delocalization is directly coupled to an increase in CT dissociation efficiency. Therefore, our results substantiate the concept of delocalization of electrons taking an important and positive role in the charge separation process.

CPP 39.4 Wed 10:30 C 243

Incoherent Pathways of Charge Separation in Organic and Hybrid Solar Cells — •Tobias Seewald, Alexander Grupp, Philipp Ehrenreich, Julian Kalb, Arne Budweg, Lukas Schmidt-Mende, and Daniele Brida — Department of Physics and Center for Applied Photonics, University of Konstanz, D-78457 Konstanz, Germany

In this work, we investigate the exciton dissociation dynamics occurring at the donor:acceptor interface in organic and hybrid blends employed in the realization of photovoltaic cells. Fundamental differences in the charge separation process are studied with the organic semiconductor polymer poly(3-hexylthiophene) (P3HT) and either [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) or titanium dioxide (TiO2) acting as the acceptor. By using ultrafast broad-band transient absorption spectroscopy with few-fs temporal resolution, we observe that in both cases the incoherent formation of free charges dominates the charge generation process. From the optical response of the polymer and by tracking the excited-state absorption, we extract pivotal similarities in the incoherent energy pathways that follow the impulsive excitation. On time scales shorter than 200 fs, we observe that the two acceptors display similar dynamics in the exciton delocalization. Significant differences arise only on longer time scales with only an impact on the overall photocarrier generation efficiency.

CPP 40: Wetting, Microfluidics and Confined Liquids I (joint session CPP/DY)

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

Invited Talk CPP 40.1 Wed 9:30 C 264

Slippage over superhydrophobic surfaces: fundamentals and local phenomena — •Clarissa Schönecker[1,2], David Schäffel[2], Kaloian Koynov[2], Doris Vollmer[2], and Hans-Jürgen Butt[2] — [1]Lehrstuhl für Mikrofluidmechanik, TU Kaiserslautern — [2]Max-Planck-Institut für Polymerforschung, Mainz

Superhydrophobic surfaces can provide a significant slip to a fluid flowing over the surface, making them attractive for the development of functional coatings. Although the global behaviour of flow past such surfaces has been widely investigated, understanding the local fundamentals that lead to slippage is still lacking. We studied in detail the local slip length and local flow field for water in the Cassie state on a structured superhydrophobic surface. Using fluorescence correlation spectroscopy, we revealed that the local slip length of a superhydrophobic surface is finite, non-constant and anisotropic. Furthermore, it can be strongly influenced by the presence of surface active substances. All these properties are in accordance with and can be explained by a theoretical model of the local hydrodynamics close to the surface. The study shows the effect of surface properties, like the surface geometry or interfacial forces.

CPP 40.2 Wed 10:00 C 264

How drops start sliding over solid surfaces — Doris Vollmer[1], Nan Gao[1,2], Florian Geyer[1], Dominik Pilat[1], Sanghyuk Wooh[1], Hans-Jürgen Butt[1], and •Rüdiger Berger[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Fudan University, 220 Handan Road, Shanghai 200433, People's Republic of China

We report that the lateral adhesion force between a liquid drop and a solid can be divided into a static and a kinetic regime. This striking analogy with solid-solid friction is a generic phenomenon that holds for liquids [1]. We have investigated the lateral adhesion forces of liquids of different polarities and surface tensions on smooth, rough and structured surfaces. The lateral adhesion forces were measured with a home build instrument [2] and calculated by the occurring changes of the rear and the front of the drop, its changes in drop widths and the liquid-air surface tension. Our studies indicate that the lateral adhesion force is dominated by contact line friction and interfacial friction only plays a minor role. Finally, the lateral adhesion force measurements can provide quantitative information on the homogeneity or cleanliness of surfaces.

References:

[1] N. Gao, F. Geyer, D.W. Pilat, S. Wooh, D. Vollmer, H.-J. Butt, R. Berger, Nature Physics (2017), doi: 10.1038/NPHYS4305

[2] D. W. Pilat, P. Papadopoulos, D. Schäffel, D. Vollmer, R. Berger, H.-J. Butt, Langmuir 28, 16812-16820(2012), doi 10.1021/la3041067

CPP 40.3 Wed 10:15 C 264

Beyond the Navier-de Gennes Paradigm: Slip Inhibition on Ideal Substrates — Mark Ilton[1,2], Thomas Salez[3,4], Paul Fowler[1,5], Marco Rivetti[5], Mohammed Aly[6], Michael Benzaquen[4,7], Joshua McGraw[1,6], Elie Raphael[4], Kari Dalnoki-Veress[1], and •Oliver Bäumchen[5] — [1]McMaster University, Hamilton, Canada — [2]University of Massachusetts, Amherst, MA, USA — [3]Univ. Bordeaux, Talence, France — [4]ESPCI Paris, Paris, France — [5]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [6]Ecole Normale Supérieure, Paris, France — [7]Ecole Polytechnique, Palaiseau Cedex, France

Hydrodynamic slip of a liquid at a solid surface governs liquid transport at small scales. For polymeric liquids, de Gennes predicted that the Navier boundary condition together with the theory of polymer dynamics imply extraordinarily large slip for entangled polymer melts on ideal surfaces; this Navier-de Gennes paradigm was confirmed using dewetting experiments on ultra-smooth, low-energy substrates. Here, we use capillary leveling of polymeric films on these same substrates to measure the slip length from a robust one-parameter fit to a lubrication model. We show that at the low shear rates involved in leveling experiments, the employed substrates can no longer be considered ideal. The data is instead consistent with physical adsorption of polymer chains at the solid/liquid interface. We extend the Navier-de Gennes description using one additional parameter, namely the density of physically adsorbed chains per unit surface. The resulting model is found to be in excellent agreement with the experimental observations.

CPP 40.4 Wed 10:30 C 264

Consistency condition for macro- and mesoscopic descriptions of contact line with surfactant — •Uwe Thiele[1], Sarah Trinschek[1], Jacco H. Snoeijer[2], and Karin John[3] — [1]Institut für Theoretische Physik, Universität Münster, Wilhelm-Klemm-Str. 9, Münster — [2]Physics of Fluids Group, Faculty of Science and Technology, University of Twente, Enschede — [3]Laboratoire Interdisciplinaire de Physique, Université Grenoble-Alpes, CNRS

Consider a three-phase contact line where a liquid-gas interface meets a solid. For a simple liquid at equilibrium it is described on the macroscale by the Young-Dupré law relating the three interfacial energies to the equilibrium contact angle θ_e. On the mesoscale, it is modelled by a film-height-dependent wetting energy $f(h)$. Macro- and mesoscale description are consistent if $\gamma\cos\theta_\mathrm{e} = \gamma + f(h_a)$ where γ and h_a are the liquid-gas interface energy and the thickness of the equilibrium adsorption layer, respectively.

Our contribution discusses the incorporation of insoluble surfactant. We derive the macro- and mesoscopic equilibrium models for spatially inhomogeneous states (consistent with the dynamic approach of [1,2]). Discussing the case of a static contact line with surfactant, we show that again there exists a consistency condition between macro- and mesoscopic descriptions. It imposes a particular dependence of the wetting energy on surfactant concentration. This is illustrated at a simple example. [1] U. Thiele, A. J. Archer and M. Plapp, *Phys. Fluids* **24**, 102107 (2012). [2] U. Thiele, A. J. Archer and L. M. Pismen, *Phys. Rev. Fluids* **1**, 083903 (2016).

15 min. break

CPP 40.5 Wed 11:00 C 264

What determines the lateral adhesion force? — •Doris Vollmer, Nan Gao, Sanghyuk Wooh, Rüdiger Berger, and Hans-Jürgen Butt — MPI für Polymerforschung, Mainz

The mobility of drops on surfaces depends on the interactions between the drop, the surface and its surrounding medium. The strength of the interactions is reflected in the lateral adhesion force, FLA. We have investigated the lateral adhesion forces of droplets of water on a superhydrophobic periodic structure made of TiO2 pillars or varying distance, using a laser deflection system. The force per pillar across the effective contact width did not change with the spacing ratio. Notably, the lateral adhesion force can be calculated, knowing either (i) the apparent contact width and the apparent contact angles or the (ii) real contact width and the contact angle on the corresponding flat surface.

CPP 40.6 Wed 11:15 C 264

Efficient Condensation and Droplet Removal on Electrowetting-Functionalized Surfaces — Davood Baratian, Ranabir Dey, Harmen Hoek, Dirk van den Ende, and •Frieder Mugele — University of Twente; Physics of Complex Fluids, Enschede, The Netherlands

Efficient condensation of vapor and collection of fog from the atmosphere are important to life in arid environments. Nature has come up with various strategies to optimize the processes by a combination of both topographic and chemical functionalization of solid surfaces that are imprinted passively into the structure of the surface. One crucial aspect in this process is the removal of liquid from the solid surface once it has condensed. In here, we present a novel active approach to improve the efficiency of vapor condensation onto hydrophobic surfaces that are functionalized by electrowetting. We fabricated electrowetting-functionalized surfaces with submerged interdigitated electrodes. Upon exposure to supersaturated vapor droplets condense onto these surfaces in an initially random pattern. As the droplets grow, electrowetting mobilizes the growing drops and induces early coalescence, giving rise to alignment of drops and to early shedding. Mobilization and early shedding are controlled by the effective reduction of contact angle hysteresis in AC electrowetting. Drops are found to grow algebraically, initially with a self-similar growth law as in conventional drop condensation. At a later stage, self-similarity is broken and the statistical drop size distribution is altered. We discuss potential applications in terms of heat transfer.

CPP 40.7 Wed 11:30 C 264

Forced dynamic dewetting of structured surfaces: Influence of surfactants — •Günter K. Auernhammer[1,4], Franziska Henrich[1], Dorota Linke[1], Hans Martin Sauer[2], Edgar Dörsam[2], Steffen Hardt[3], and Hans-Jürgen Butt[1] — [1]MPI Polymer Research, Mainz, Germany — [2]TU Darmstadt, IDD, Germany — [3]TU Darmstadt, Nano- und Mikrofluidik, Germany — [4]IPF, Dresden

We investigate dynamic dewetting on structured surfaces. The focus lies on the interplay between surface structure and surfactants concentration in forced dewetting. The structured surfaces are printing plates for gravure printing with different sizes of the gravure cells. These plates were mounted on a rotating horizontal cylinder that is half-immersed in an aqueous solution of the anionic surfactant sodium 1-decanesulfonate. On the printing plates, structured and unstructured areas were side by side to enable a direct comparison. When rotating the cylinder a liquid meniscus is partially drawn out of the liquid. The moving contact line was pinned on the borders of the gravure cells, leading to a strongly varying receding contact angle. For this reason we compare the height differences of the meniscus on the structured and unstructured area. With increasing size of the gravure cells this height difference increases. By adding surfactant, the height difference for the same surface decreases. We conclude that the surfactant reduces the influence of a structured surface on dynamic dewetting. Characterizing the emptying mechanism of the gravure cells revealed that some liquid is left in the gravure cell.

CPP 40.8 Wed 11:45 C 264

Spatially Resolved NMR with Micrometer Resolution in Static Field Gradients — •Benjamin Kresse, Mark Höfler, Alexei F. Privalov, and Michael Vogel — TU Darmstadt, Hochschulstr. 6, 64289 Darmstadt, Germany

A new probe head is presented which is specially designed for magnetic resonance imaging (MRI) with ultrahigh resolution in one dimension using a static field gradient magnet. In contrast to clinical MRI scanners with a spatial resolution of typically 0.1 to 1 mm a resolution of about $2\,\mu$m is reached due to the high field gradient of 73 T/m. Systems with a rotational symmetry can be investigated by scanning the sample slice-wise. The key feature of the probe is a precise computer controlled adjustment of the sample position and orientation e.g. to adjust the sample axis parallel to the gradient of the magnetic field.

Wetting processes can be investigated. For example, droplets on surfaces can be studied in terms of density by inspecting the signal amplitude and in terms of molecular dynamics by measuring the relaxation time of the nuclear spins. Furthermore, concentration gradients of mixtures can be examined by measurements on different isotopes. It is also possible to investigate biological objects with flat geometries like skin. In principle non-stationary processes like in microfluidics can be explored with an increased time resolution by a boosted signal-to-noise ratio using stripline designs.

CPP 40.9 Wed 12:00 C 264

Feedback-Control of Photoresponsive Fluid Interfaces — •Josua Grawitter and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Deutschland

New microfluidic devices promise powerful applications in diagnosing and combatting illness around the world. Conventional, pressure-driven devices rely on static channel geometries designed for specific flow patterns. Light-driven devices instead use photosensitive surfactants to produce surface tension gradients that drive Marangoni currents. By changing their light patterns in response to fluid flow, light-driven devices add feedback control methods to the microfluidic toolbox.

To explore their potential, we develop a diffusion-advection-reaction equation for photosensitive surfactants and calculate Marangoni currents at fluid-fluid interfaces. We then study how the interface responds when illuminated by spots of light. Switching on a single light spot, the density of the switched surfactant spreads in time and assumes an exponentially decaying profile in steady state. Simultaneously, the induced radial Marangoni flow reverses its flow direction from inward to outward. We use this feature to set up specific feedback rules, which couple advection velocities sensed at the light spots to their intensities. As a result two neighboring spots switch on and off alternately. When we arrange more light spots on regular polygons, regular and irregular oscillations in light intensity emerge for certain numbers of spots. This demonstrates how light-driven feedback control may be used to create responsive and versatile microfluidic devices.

CPP 40.10 Wed 12:15 C 264

Collective Orientational Order and Phase Behavior of a Discotic Liquid Crystal under Confinement — •Arda Yildirim[1], Kathrin Sentker[2], Patrick Huber[2], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — [2]Institut für Materialphysik und -technologie, Technische Universität Hamburg, Eißendorfer Str. 42, 21073 Hamburg, Germany

Discotic liquid crystals (DLCs) are a promising class of soft matter for electronic applications. This is due to their ability to self-organize into columns in a hexagonal columnar mesophase, driven by the overlapping of the π orbitals of their aromatic cores. This leads to a high charge-carrier mobility along the column axis. Previous studies on DLCs showed that their properties, such as phase transition temperatures and enthalpies, are susceptible to nanoconfinement [1,2]. In this study, 2,3,6,7,10,11 hexakis[hexyloxy] triphenylene (HAT6) was confined into parallel aligned cylindrical nanopores of anodic aluminum oxide (AAO) membranes by melt infiltration. Furthermore, the pore surfaces of a series of membranes were chemically modified, resulting in a more hydrophobic pore surface than the unmodified ones. Collective orientational order and phase behavior of HAT6 confined into modified and unmodified nanopores of AAO were investigated by broadband dielectric spectroscopy and differential scanning calorimetry respectively.

[1] C. Krause and A. Schönhals, J. Phys. Chem. C, 2013, 117, 19712.

[2] C. Krause et al., Colloid Polym. Sci., 2014, 292, 1949

CPP 40.11 Wed 12:30 C 264

Reversible smectic layer buckling of a ferroelectric liquid crystal confined in anodic aluminium oxide nanochannels — •Mark Busch[1], Andriy V. Kityk[2,1], Tommy Hofmann[3], Dirk Wallacher[3], and Patrick Huber[1] — [1]TU Hamburg-Harburg, Hamburg, Germany — [2]Czestochowa University of Technology, Czestochowa, Poland — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

The temperature-dependent structural and electro-optical properties of the ferroelectric liquid crystal 2MBOCBC inside the confining cylindrical nanochannels of anodic aluminium oxide are investigated.[1] The channel walls of the 42 nm diameter pores are coated with a polymer to enforce a planar anchoring of this chiral mesogens. By means of neutron diffraction a fully reversible temperature-dependent smectic C* layer buckling towards a symmetric chevron-like structure is found. The formation of this structure coincides with a dramatic decrease in the linear electro-optical response, being explained by the aforementioned structural rearrangement.

[1] Busch et al., Nanoscale (2017), DOI: 10.1039/C7NR07273B

CPP 40.12 Wed 12:45 C 264

Transport processes in water vapour sorption experiments on grained hygroscopic materials — •Alexander Murr — Institute for Structural Engineering and Material Science, University of Innsbruck

Water vapour sorption (WVS) experiments are frequently used to characterise the behaviour of hygroscopic materials for a variation in humidity. Sample material is exposed to a step change in relative humidity (RH) and the mass change is measured gravimetrically.

In order to identify the involved transport processes, WVS experiments on grained wood and cellulose have been performed. A comparison on the sorption kinetics of four different grain layer filling levels indicates the necessarity of including the water vapour transport between the sample surface and the forced air stream. Analysing the initial kinetics shows this transport being relevant for the whole range of RH. Additionally, the limitation of a non-instantaneous step change in RH will be discussed. An analysis based on a simple diffusion equation with an instantaneous sink provides further insights on the measured sorption kinetics. Consequently, the relaxation and reorganisation processes could be more easily separated and characterised in future experiments.

CPP 41: Networks (joint session SOE/DY/BP) (joint session SOE/CPP/BP/DY)

Time: Wednesday 9:30–12:15 Location: MA 001

CPP 41.1 Wed 9:30 MA 001

Dynamics of interacting tipping elements on complex networks — •Jonathan F. Donges[1,2], Ann-Kristin Klose[1], and Ricarda Winkelmann[1] — [1]Earth System Analysis, Potsdam Institute for Climate Impact Research, Potsdam, Germany — [2]Stockholm Resilience Centre, Stockholm University, Stockholm, Sweden

In recent years, an increasing number of potential tipping elements have been identified in ecological, climatic and social systems. Tipping elements are defined by their ability to undergo large qualitative change that is caused by a small perturbation in a parameter or state variable. We investigate the emergent nonlinear dynamics of pairs, chains and networks of generalized tipping elements. Understanding the dynamics of systems of interacting tipping elements on complex networks is relevant for assessing the resilience and transformative capacity of complex systems such as the Earth's climate system and the World's energy system in the context of decarbonization transformation for meeting the Paris climate agreement.

CPP 41.2 Wed 9:45 MA 001

The interdependent network of gene regulation and metabolism is robust where it needs to be — •Marc Hütt[1], David Klosik[2], Anne Grimbs[1], and Stefan Bornholdt[2] — [1]Jacobs University, Bremen, Germany — [2]Institute for Theoretical Physics, University of Bremen, Bremen, Germany

Despite being highly interdependent, the major biochemical networks of the living cell – the networks of interacting genes and of metabolic reactions, respectively – have been approached mostly as separate systems so far. Recently, a framework for interdependent networks has emerged in the context of statistical physics. In a first quantitative application of this framework to systems biology, here we study the interdependent network of gene regulation and metabolism for the model organism *Escherichia coli* in terms of a biologically motivated percolation model [1]. Particularly, we approach the system's conflicting tasks of reacting rapidly to (internal and external) perturbations, while being robust to minor environmental fluctuations. Considering its response to perturbations that are localized with respect to functional criteria, we find the interdependent system to be sensitive to gene regulatory and protein-level perturbations, yet robust against metabolic changes. We expect this approach to be applicable to a range of other interdependent networks.

[1] Klosik, D. F., Grimbs, A., Bornholdt, S., and Hütt, M.-T. (2017). Nature Communications, 8(1):534.

CPP 41.3 Wed 10:00 MA 001

Robust connectivity in networks with groups of vulnerable nodes — •Sebastian M. Krause[1,2], Michael M. Danziger[3], and Vinko Zlatić[2] — [1]Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany — [2]Theoretical Physics Division, Rudjer Bošković Institute, Bijenicka c. 54, 10000 Zagreb, Croatia — [3]Department of Physics, Bar-Ilan University, Ramat Gan 5290002, Israel

In many networked systems there are large groups of similar nodes which are vulnerable to the same failure or adversary. For example, servers in a communication network running the same software will fail together, if this software has a bug. Therefore, we are often faced with networks where all nodes of a group can fail together. Further, many different vulnerabilities can cover the whole network. This structural weakness has so far been overlooked in studies of network robustness. Here we discuss, how multiple redundant paths enable a high level of robustness, even if no node is trusted [1,2]. With each vulnerability described as a color, we discuss "color-avoiding percolation". We present a fast numerical algorithm for real world networks and analytical results for random network ensembles.

[1] Sebastian M. Krause, Michael M. Danziger, and Vinko Zlatić, Hidden Connectivity in Networks with Vulnerable Classes of Nodes, Phys. Rev. X 6, 041022 (2016).

[2] S. M. Krause, M. M. Danziger, and V. Zlatić, Color-avoiding percolation, Phys. Rev. E 96 022313 (2017).

CPP 41.4 Wed 10:15 MA 001

When is a network a network? Multi-order graphical model selection in time series data on networks — •Ingo Scholtes — Chair of Systems Design, ETH Zürich, Zürich, Switzerland

We introduce a novel framework for the modeling of time series data on networks. Such data are important, e.g., when studying click streams of users in the Web, travel patterns of passengers in transportation systems, information cascades in social networks, biological pathways, or time-stamped social interactions. While it is common to apply graph analytics and network analysis to such data, recent works have shown that temporal correlations can invalidate the results of such methods. This raises a fundamental question: When is a network abstraction of time series data justified?

Addressing this open question, we propose a framework that combines Markov chains of multiple, higher orders into a multi-layer network model that captures temporal correlations at multiple length scales simultaneously. We develop a model selection technique to infer the optimal number of layers of such a model and show that our method outperforms baseline Markov order detection techniques.

An application to eight real-world data sets capturing causal paths in time series data on networks shows that the inferred models provide an optimal summarization of the causal topologies of real-world complex systems. Our work highlights fallacies of network-based modelling techniques and provides a principled answer to the open question when they are justified. Generalizing networks to optimal multi-order models, it opens perspectives for the study of complex systems.

CPP 41.5 Wed 10:30 MA 001

Exact expected cluster sizes for bond percolation in finite networks — Joan Pont Serra and •Konstantin Klemm — IFISC (CSIC-UIB), Mallorca, Spain

Bond percolation describes the statistical ensemble generated by randomly deleting edges from a given network. Traditionally studied on grids (lattices), bond percolation forms a crucial part of modern network theory with implications for epidemic spreading and network robustness under failures. For quenched systems of size well above 20 nodes, the computation of percolation quantities relies on heuristics (e.g. by the graph spectrum) or Monte Carlo sampling. Here we introduce an exact computational method that is time-efficient when the network has certain separation properties. Specifically, we work with a branch decomposition of low width. Then the network is recursively separable by removing a small number of nodes in each step. For several test networks, we present exact results for the first time. We find that the computational cost of our exact method is lower than that of Monte Carlo runs required to reach an acceptable precision.

CPP 41.6 Wed 10:45 MA 001

Controlling percolation with limited resources — •Malte Schröder[1], Nuno Araújo[2], Didier Sornette[3], and Jan Nagler[3] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Universidade de Lisboa, Lisboa, Portugal — [3]ETH Zürich, Zurich, Switzerland

Connectivity - or the lack thereof - is crucial for the proper functioning of many essential socio-economic processes, from financial and economic networks over epidemic spreading in social networks to technical infrastructure. Often, connections are deliberately established or removed by various parties to induce, maintain, or destroy global connectivity. Thus, there has been a great interest in understanding how to control percolation, the transition to large-scale connectivity. Previous work studied control strategies implicitly assuming unlimited resources, leading to a large number of models of "explosive" and discontinuous percolation. Realistically, however, such control is often subject to a limited budget. We derive an efficient control strategy to delay percolation under the constraint of limited resources and study its implications. We show that the transition can be significantly delayed even with scarce resources but remains smooth and in the same universality class as random percolation. In particular, the transition never becomes "explosive". We derive an approximation for the optimal control parameters and show how resource optimal delay of percolation leads to a sudden, discontinuous transition. Thus, the percolation transition becomes effectively uncontrollable as an unintended consequence of optimal control.

CPP 41.7 Wed 11:00 MA 001

Discrete reaction-diffusion models of innovations using multi-particles in networks. — •Yuki Kawasaki and Hirotada Ohashi — The University of Tokyo, Tokyo, Japan

Reaction-diffusion is a fundamental process underlying many social and economic phenomena. This process has been widely studied in continuous physical space. Different from physical and chemical phenomena, social and economic processes occur in networks connecting individuals, firms and organizations. In this study, we model reaction-diffusion processes of innovations in structured networks employing multi-particles that represent innovations and some kind of enzymes. The reaction process is that several particles react on nodes according to reaction rules and the diffusion process is that particles travel randomly to neighboring nodes. This model is able to reproduce macroscopic behaviors of systems taking account of microscopic relationships between individual particles. Simulation results are obtained for various network structures including small-world and scale-free networks. Next we extend our model to deal with simultaneous reaction and diffusion of different kinds of particles. This model can describe competition and cooperation between innovations in networks including predator-prey processes.

CPP 41.8 Wed 11:15 MA 001

Probabilistic Quantifiers for Deterministic Spreading — •Justine Wolter[1,2], Benedict Lünsmann[3], Xiaozhu Zhang[1,2], Malte Schröder[1,2], and Marc Timme[1,2,3] — [1]Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), TU Dresden, Dresden, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen — [3]Max Planck Institute for the Physics of Complex Systems, 01069 Dresden

How do signals spread across dynamical systems? Spreading may be stochastic, e.g., during epidemic outbreaks or deterministic, e.g., in electrical or other supply networks. Due to mathematical challenges, it remains unknown how to robustly quantify even simple characteristics such as peak times or amplitudes of a spreading signal propagating across a network. Here we change the perspective and propose to analyze deterministic spreading dynamics employing concepts of probability theory. We characterize generic spreading dynamics by expectation values to work out a theory explicitly quantifying when and how strongly a perturbation initiated at one unit of a network impacts any other [1]. The theory provides this information as a function of the relative position of initially perturbed and responding unit as well as on the entire network topology. Furthermore, asymptotically exact approximation schemes enable to well predict previously inaccessible peak times and amplitudes. These insights may open up a new realm of quantifying characteristics of deterministic processes through probability theory. Ref.: [1] J. Wolter et al., http://arXiv.org/abs/1710.09687

CPP 41.9 Wed 11:30 MA 001

Perturbation spreading on diffusively-coupled networks and power grids — •Xiaozhu Zhang[1,2], Dirk Witthaut[3], and Marc Timme[1,2] — [1]Chair for Network Dynamics, Institute for Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), TU Dresden, Dresden, Germany — [2]Network Dynamics, Max Planck Institute for Dynamics and Self-organization, 37077 Göttingen — [3]Institute for Energy and Climate Research - Systems Analysis and Technology Evaluation (IEK-STE), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Spreading phenomena on networks essentially underlie the collective dynamics of systems across physics, biology and engineering. Yet, how local changes dynamically spread in such networked systems is still far from fully understood. Here we analyze the spreading dynamics for diffusively-coupled networks close to given operating points. We provide analytical solutions of transient nodal responses via linear response theory and approximate the perturbation arrival times via Taylor expansion. In homogeneous networks, we find the spreading speed based on the estimated arrival times decreases and converges to a constant at large distance. Intriguingly, the asymptotic spreading speed is essentially determined by the network topology, i.e. the limiting behavior of the number of shortest paths at large distance. These results shed light on the qualitatively universal asymptotic spreading behavior in networks and its quantitative dependence on the underlying network topology.

CPP 41.10 Wed 11:45 MA 001

Temporal networks with geometric constraints and protein folding — •Nora Molkenthin[1], Marc Timme[2,1], and Steffen Mühle[3] — [1]Network Dynamics, Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen — [2]Chair for Network Dynamics, Center for Advancing Electronics Dresden (cfaed) and Institute for Theoretical Physics, TU Dresden, 01062 Dresden — [3]Physics Department III, University of Göttingen, D-37077 Göttingen, Germany

The structure of many complex networks is highly constrained by geometric factors, affecting a broad range of systems from polymer aggregates to traffic and supply networks. On the microscopic scale, folding proteins constitute paradigmatic systems for spatial network formation. They are well characterized as Protein Residue Networks (PRN) yet their statistical properties seem to be diverse and general rules are largely unknown. Here, advancing a recent graph-theoretical mapping [1], we develop a temporal network model for the aggregation of connected, spatially extended units, thereby reproducing key features of PRN*s. In stark contrast to network models without geometric constraints, we observe algebraic scaling of the network diameter with system size and predict the characteristic link length distribution, both features fitting with those experimentally observed in PRN*s.

[1] Molkenthin & Timme, Scaling Laws in Spatial Network Formation, Phys. Rev. Lett. 117:168301 (2016)

CPP 41.11 Wed 12:00 MA 001

Non-inertial reference frames for inferring networks from dynamics — •Jose Casadiego[1,2] and Marc Timme[1,2] — [1]Chair for Network Dynamics, Institute of Theoretical Physics and cfaed - Center for Advancing Electronics Dresden, Technical University of Dresden, Dresden, Germany — [2]Network Dynamics, Max Planck Institute for Dynamics and Self-Organization (MPIDS), Goettingen, Germany

The dynamics of complex networks are determined to a great extent by the connectivity of their units. Given that measuring the connectivity by direct methods is often infeasible, researchers typically apply inverse approaches to infer links between units from the collective dynamics. Current state-of-the-art methods rely on either (i) quantifying functional links through statistical dependencies, or (ii) approximating the possibly nonlinear interactions between units via modeling of differential equations. Yet, functional links frequently do not match physical links, and finding an appropriate model may be computationally demanding and also require a prior knowledge about the interactions. Here we develop a model-independent theory to reconstruct the connectivity of networks from transients states to stable dynamics. Specifically, we demonstrate that representing these transients with respect to non-inertial reference frames provides simple linear mappings between network connectivity and dynamics. Furthermore, we show the robustness of our framework by reconstructing the full connectivity of different network dynamical systems exhibiting phase-locking, periodic orbits and collective synchronization.

CPP 42: Materials for Energy Storage I (joint session KFM/CPP)

Organizer: Martin Diestelhorst - Martin-Luther-Universität Halle-Wittenberg - Halle

Time: Wednesday 9:30–12:30 Location: EMH 025

Invited Talk CPP 42.1 Wed 9:30 EMH 025

Resource-efficient dielectric materials for short-time energy storage — •Stephan Krohns — Experimental Physics V, University of Augsburg, 86159 Augsburg

Materials exhibiting so-called colossal effects have an enormous potential for future use in correlated electronics, including capacitors for energy storage. The search for functional dielectrics showing colossal dielectric constants (CDC) is still an active field of research [1].

Beside the pure materials properties, also the scarcity and possible future shortages of used key elements in this modern technology is in the focus of scientific interest. An imminent challenge of modern materials science is the development of materials with less critical elements that have comparable or better functionalities than those currently used.

In this talk, I address the pure materials science perspective focusing on the research of CDC materials like crystals showing barrier layer capacitances [2] as well as ionic liquids. The latter are promising candidates for electrolytes used in supercapacitors [3]. Furthermore, I present a practical guideline for basic research implementing resource strategy aspects [4] as well as a possible scenario for the system and market integration of those short-term energy storages [5].

[1] S. Krohns et al., Nat. Mat. 10, 899 (2011).
[2] E. Ruff et al., Phys. Rev. Lett. 118, 036803 (2017).
[3] P. Sippel et al., Sci. Rep. 5, 13922 (2015).
[4] Ch. Helbig et al., Sust. Mat. & Techn. 12, 1 (2017).
[5] M. Hassler et al., OR Spectrum 38, 633 (2016).

CPP 42.2 Wed 10:00 EMH 025

Dielectric properties of ionic liquid based electrolytes for future energy-storage systems — •Pit Sippel and Stephan Krohns — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

Electrolytes are essential for energy storage systems like electric double layer capacitor (EDLC). The so-called electrode polarization is the driving mechanism for energy storage in EDLCs. To enhance the properties of EDLCs, potential new electrolytes are investigated by various methods. Dielectric spectroscopy is a powerful tool analyzing the electric properties of liquids. This technique allows measuring the relaxation times of dynamic processes and ionic conductivity in a broad frequency and temperature range. Especially, the ionic conductivity is an essential figure of merit for any energy-storage application. This talk addresses the dielectric properties of ion conducting liquids with special emphasize put on ionic liquids (ILs). The revealed spectra are analyzed using equivalent circuits, which enable investigating the important electrode polarization effect. ILs offer outstanding properties (e.g., low volatility and high electrochemical stability) making them promising candidates for solvent-free electrolytes, which may improve energy-storage systems. However, the applicability of ILs is still hampered due to their rather low conductivity. We address the question if this conductivity can be optimized by mixing pure ILs taking into account the non-canonical super-Arrhenius temperature dependence [1].
[1] E. Thoms *et al.*, Sci. Rep. **7**, 7463 (2017).

CPP 42.3 Wed 10:20 EMH 025

Influence of the glass-ceramic synthesis route on the ionic conductivity of the sodium solid electrolyte $\mathbf{Na_2O\text{-}Y_2O_3\text{-}SiO_2}$

— •Wolfram Münchgesang[1], Dörthe Wagner[2], Mykhaylo Motylenko[3], Jochen Schilm[2], David Rafaja[3], and Dirk C. Meyer[1] — [1]Institut für Experimentelle Physik, Technische Universität Bergakademie Freiberg, 09599 Freiberg, Germany — [2]Fraunhofer-Institut für Keramische Technologien und Systeme IKTS, 01277 Dresden, Germany — [3]Institut für Werkstoffwissenschaft, Technische Universität Bergakademie Freiberg, 09596 Freiberg, Germany

The development of room-temperature solid electrolytes (SEs) is one of the keys for the realization of solid-state batteries – a post lithium-ion technology, with probably better performance than this. For SEs, a glass-ceramic synthesis route (GCSR) is particularly suitable, because this is less expensive than other production methods and can be used on an industrial scale.

The maximum achievable conductivity (C) of SEs is determined by the used ionic-conductive phase (ICP), which is crystalline $Na_5YSi_4O_{12}$ in our case. In practice C is strongly influenced by the microstructure of the SE, in particular by the formation of a suitable percolation path; which is determined by the ratio of the ICP and its crosslinking. We will present the influence of different GCSRs on the microstructure of the SE and the resulting conductivity change.

This work was financed by the Federal Ministry (FM) of Education and Research within the project SyNeSteSia (05K14OFA) and the FM for Economic Affairs and Energy within the project BaSta (0325563).

CPP 42.4 Wed 10:40 EMH 025

Water Adsorption on a n-Si/NiO Photoanode - Cryo Photoelectron Spectroscopy in the Frozen Electrolyte Approach — •Mathias Fingerle, Sven Tengeler, Wolfram Calvet, Thomas Mayer, and Wolfram Jaegermann — Surface Science Division, Department of Materials Science, Technical University Darmstadt, Otto-Berndt-Str. 3, D-64287 Darmstadt, Germany

In the course of the BMBF InnoEMat project Fundamentals of Electrochemical Interfaces: Semiconductor/Electrolyte, elemental charge transfer processes at solid/liquid interfaces are studied via cryo photoelectron spectroscopy and post-operando experiments. Here, the interaction of water with a magnetron-sputtered nickel oxide thin film on an n-type silicon photo-anode is investigated in perspective to oxygen evolution. The substrate was exposed in-situ stepwise to gas phase water up to 10 L at liquid N2 temperature and analyzed via X-ray and UV photoelectron spectroscopy in the so called frozen electrolyte approach. Photoemission of the pristine NiOx layer shows the presence of stoichiometric NiO and Ni2O3 as well as of non-stoichiometric phases. In the monolayer range, molecular and dissociative adsorption is detected assigned to the NiO respective Ni2O3 phase. Initially, the emissions of the molecular adsorbed water species interacting with NiO are found at 0.8 eV lower binding energies as compared to water related emissions for higher coverages with binding energies commonly assigned to H2O-H2O interaction. In addition to the chemical analysis, the electronic structure of the n-Si/SiOx/NiOx/H2O photoanode is measured and discussed.

20 min. break

CPP 42.5 Wed 11:20 EMH 025

Morphologischer Einfluss von BaTiO3 Partikeln auf die Leitfähigkeit und Speicherzeit von Oxid*Polymer-Filmkondensatoren — •Sandra Wickert[1], Till Mälzer[2], Frank Apsel[3], Tino Band[4], Hartmut Leipner[5], Martin Diestelhorst[6] und Stefan Ebbinghaus[7] — [1]enfas GmbH, D-80809 — [2]enfas GmbH, D-80809 — [3]enfas GmbH, D-80809 — [4]Institut für Physik, MLU Halle-Wittenberg, D6120 — [5]IZM, MLU Halle-Wittenberg, D6120 — [6]Institut für Physik, MLU Halle-Wittenberg, D6120 — [7]Institut für Chemie, MLU Halle-Wittenberg, D6120

Der Einfluss der Morphologie von BaTiO3 Partikeln auf die Leitfähigkeit und die daraus resultierende Speicherzeit von BaTiO3/P(VDF-HFP)-Folienkondensatoren wurde untersucht. Dazu wurden über die Mischoxidsyntheseroute BaTiO3*Partikel unterschiedlicher Form und Größe hergestellt und in Lösungen des ferroelektrischen Polymers P(VDF-HFP) suspendiert. Über eine Rakelanlage wurden diese Lösungen in Folien gegossen und nach verschiedenen Verfahren getrocknet. Nach Kontaktierung erfolgte die dielektrische Auswertung der so erhaltenen Kondensatoren mittels unipolarer zyklischer Polarisationsmessungen. Es konnte gezeigt werden, dass sowohl die Größe als auch die Form der BaTiO3-Partikel eine entscheidende Rolle für die Gesamtleitfähigkeit des Systems spielen. Außerdem konnte das bisherige core-shell-Modell für die Bildung von BaTiO3 erweitert werden, so dass nicht nur die Entstehung der Einzelpartikel beschrieben wird, sondern auch die Bildung von Agglomeratstrukturen erklärt werden kann.

CPP 42.6 Wed 11:40 EMH 025

Investigation of electrical conductivity and dielectric properties in ceramic-polymer composite films — •Till Mälzer[1,4], Tino Band[2], Sandra Wickert[3,5], Frank Apsel[1,5], Hartmut S. Leipner[1], Martin Diestelhorst[2], and Stefan Ebbinghaus[3] — [1]Center of Materials Science, Martin-Luther-University Halle-Wittenberg (MLU), 06120 Halle (Saale) — [2]Department of Physics, MLU — [3]Department of Chemistry, MLU — [4]enfas GmbH, 86668 Karlshuld — [5]enspring GmbH, 06120 Halle (Saale)

Dielectric materials with high energy storage density are of great importance for power electronics. Ceramic-polymer composites have been evaluated as a candidate for dielectric materials for new-type capacitors, due to the possibility to tailor materials properties by proper design for specific applications. Besides dielectric properties in majority of studies, the electrical conduction of the ceramic-polymer composite films has been disregarded. We report on results of composite films consisting of the two ferroelectric materials P(VDF-HFP) as polymer matrix and BaTiO3 as filler, each known for its high permittivity in its particular material class. Composite films with different size and concentration of BaTiO3 particles were fabricated via a solution cast doctor blade method. We studied the influence of particle size, agglomeration, particle distribution and filler concentration on electrical conductivity and the dielectric properties energy density, permittivity and breakdown strength of the composite films. We used charge-voltage measurements for dielectric investigations and for morphological studies X-ray diffraction and scanning electron microscopy.

Invited Talk CPP 42.7 Wed 12:00 EMH 025

Dielectric Polymer Nanocomposites for Electrical Energy Storage — •Qing Wang — The Pennsylvania State University

The demand for high-performance dielectric materials arises from numerous emerging energy storage and conditioning applications such as electric vehicles, wind generators, solar converters, and aerospace power systems. This talk will describe our most recent efforts to develop the dielectric polymer nanocomposites for capacitive energy storage applications. Specifically, the introduction of boron nitride nanosheets (BNNSs) into the polymers yields significantly reduced high-field loss and improved thermal conductivity, giving rise to great improvements in the charge-discharged efficiency and discharged energy density at high temperatures. The sandwich-structured composites with BNNSs spreading throughout the outer polymeric layers and high-dielectric-constant nanoparticles in the interior layer has been designed and experimentally demonstrated. More recently, chemical-vapor-deposited hexagonal boron nitride (h-BN) has been coated onto the surface of the polymer films. The h-BN-coated polymer films are capable of operating with >90% efficiencies and delivering high energy densities even at a temperature close to the glass transition temperature of polymer. Challenges along with future research opportunities will also be discussed.

CPP 43: Membranes and Vesicles I (joint session BP/CPP)

Time: Wednesday 9:30–13:00 Location: H 1028

CPP 43.1 Wed 9:30 H 1028

Actin polymerization driving localized membrane deformation — •Remy Kusters[1], Camille Simon[1], Jean-Francois Joanny[1,2], Cecile Sykes[1], and Pierre Sens[1] — [1]Institut Curie, Paris, France — [2]ESPCI, Paris, France

The actin cytoskeleton is able to exert both pushing and pulling forces on the cell membrane, mediating processes such as cellular motility, endocytosis and cytokinesis. In order to investigate the exclusive role of actin dynamics on membrane deformations, the actin dynamics is reconstituted on the outer surface of a deformable liposome. Depending on the elasticity of the membrane and the forces generated by the actin polymerization, both tubular extrusions (i.e. towards the actin cortex) and localized spike-like protrusions occur along the surface of the liposome. In this talk I present a theoretical model where uniform actin polymerization can drive localized membrane deformations and show how polymerization kinetics and membrane/cortex mechanics impact their size and stability.

CPP 43.2 Wed 9:45 H 1028

Modeling the flat-to-curved transition during clathrin-mediated endocytosis — •Felix Frey[1], Delia Bucher[2], Kem Sochacki[3], Justin Taraska[3], Steeve Boulant[2], and Ulrich Schwarz[1] — [1]Institute for Theoretical Physics, Heidelberg University — [2]Department of Infectious Diseases, Virology, University Hospital Heidelberg — [3]NIH, Bethesda, U.S.A.

Clathrin-mediated endocytosis (CME) is essential for the cellular uptake of nutrients and receptors. Although CME has been studied for decades, the exact sequence of molecular and structural events remains elusive. Two basic models have been suggested for the way CME proceeds. (1) In the constant curvature model, it is assumed that clathrin-coated pits grow with constant curvature, determined by the geometry of clathrin triskelia. (2) In the constant area model, it is assumed that clathrin triskelia first assemble into flat hexagonal arrays that later invaginate with a constant surface area. This second model implicitly assumes that during bending, some hexagons are converted into pentagons. Here, we integrate data sets from correlative electron and light microscopy and quantify the sequence of ultrastructural rearrangements of the clathrin coat during endocytosis in mammalian cells with the help of some simple mathematical growth laws. Our analysis shows that clathrin-coated structures initially grow flat but start to acquire curvature when 70% of the final clathrin content is reached. Hence, our analysis suggests that elements of both suggested models are present and that mechanical and cellular factors will decide about the relative weights of growth versus curvature formation.

CPP 43.3 Wed 10:00 H 1028

Formation and Stabilization of Pores in Bilayer Membranes by Peptide-like Amphiphilic Polymers — •Ankush Checkervarty[1,2], Marco Werner[1,3], and Jens Uwe Sommer[1,2] — [1]Leibniz-Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden, Germany — [2]Institute of Theoretical Physics, Technische Universitat Dresden, Germany — [3]Universitat Rovira i Virgili, Departament dEnginyeria Quimica, Av. Paisos Catalans 26, 43007 Tarragona, Spain

We study pore formation in models of lipid-bilayer membranes interacting with amphiphilic copolymers mimicking anti-microbial peptides using Monte Carlo simulations rationalized by a simple brush-model for the fluid membrane. In our study at least a weak tension on the membrane is required to observe pore-formation induced by the adsorption of flexible amphiphilic copolymers. The copolymers enhance the pore stability by decreasing the line tension due to weak adsorption along the rim of the pore. Pore formation is enhanced with increasing length of copolymers or stronger stretching of the membrane. Both solvent and copolymer permeability increase as the pore becomes stable. Pore-formation proceeds via a meta-stable pore-state according to adiscontinuous phase transition scenario which lead to finite pore-sizes at once. Our generic model of copolymer-induced pore-formation does not require high polymer concentration at the pores nor any self-organization of the copolymers to open the pore.

CPP 43.4 Wed 10:15 H 1028

Shapes of red blood cell doublets — •Masoud Hoore, Dmitry A. Fedosov, and Gerhard Gompper — Theoretical Soft Matter and Biophysics, Institute of Complex Systems, Forschungszentrum Juelich GmbH

Red blood cell (RBC) aggregates play an important role in determining blood rheology. RBCs in solution interact attractively to form various shapes of RBC doublets. Here, the attractive interactions can be varied by changing the solution conditions. A systematic numerical study on RBC doublet formation is performed, which takes into account the shear elasticity of the RBC membrane due to the spectrin cytoskeleton, in addition to the bending rigidity. The results are obtained from molecular dynamics simulations of triangulated surfaces considering thermal effects. The phase space of the RBC doublet shapes in a wide range of adhesion strengths, reduced volumes, and shear elasticities is obtained. Experimental images of RBC doublets in different solutions show similar configurations. Furthermore, it is shown that rouleau formation is affected by the doublet structure. It is shown that the shear elasticity of the RBC membrane changes the doublet phases significantly.

CPP 43.5 Wed 10:30 H 1028

Conditions of Spontaneous Translocation of Individual Nanotube Porin Through a Phospolipid Bilayer — Yachong Guo[1,2], Marco Werner[2], Ralf Seemann[3], Vladimir Baulin[2], and •Jean-Baptiste Fleury[3] — [1]Nanjing University, Nanjing , China — [2]Universitat Rovira i Virgili, Tarragona, Spain — [3]Saarland Univsersity, Saarbruecken, Germany

Single ultra-short nanotubes can be inserted in cell membrane to be used as a membrane nanosensor or to form artificial ionic channels. Recent studies reported that ultra-short nanotubes can passively be inserted perpendicularly to the lipid bilayer core. After this insertion, it is commonly expected that these ultra-short nanotubes should stay trapped into the lipid bilayer core as its represents a potential well. In contrast to such expectations, we investigate the possible conditions that could lead a single nanotube to translocate spontaneously across a lipid bilayer. We demonstrate that membrane stretching and subnanometer nanotube, are essential to enable this type of translocation, while no translocations are occurring in lipid bilayers under low tension. The proof of this tension-dependent translocation event is obtained by observating directly a single nanotube quitting a highly stretched lipid bilayer. A quantitative analysis of the kinetic pathway associated to this translocation event is measured by using a specially designed microfluidic device combining optical fluorescence microscopy with simultaneous electrophysiological measurements.

CPP 43.6 Wed 10:45 H 1028

Membrane fluctuations of malaria-infected red blood cells — •Julia Jäger[1,2], Benjamin Fröhlich[3], Motomu Tanaka[3], Michael Lanzer[4], and Ulrich Schwarz[1,2] — [1]Institut für Theoretische Physik, Universität Heidelberg — [2]Bioquant, Universität Heidelberg — [3]Institut für Physikalische Chemie, Universität Heidelberg — [4]Parasitologie, UniversitätsKlinikum Heidelberg

Once inside the body, malaria parasites invade red blood cells in order to hide from the immune system and to digest hemoglobin. Over the course of 48 hours the parasite completely remodels the red blood cell, so that the cell becomes round and stiff and eventually breaks open. One way to monitor this remodeling process is the measurement of the cell membrane's flickering spectrum, which is a standard approach to extract the mechanical properties of cell membranes. In addition to the usual interface Hamiltonian for the membrane, we take into account the connections between the outer lipid bilayer and the spectrin network underlying the plasma membrane, which are known to become increasingly clustered over the course of the infection. We focus on the confinement parameter in the interface Hamiltonian and show how it scales with the number and strength of the connections. Finally, we compare our results with experiments.

15 min. break

Invited Talk CPP 43.7 Wed 11:15 H 1028

Computer simulation of collective phenomena that alter the topology of membranes — •Marcus Müller — Georg-August-Universität Göttingen, Institut für Theoretische Physik, Göttingen, Germany

Using computer simulation and self-consistent field theory of coarse-grained models for lipid membranes, we study the free-energy landscape of collective phenomena that alter the topology of lipid membranes. These basic processes - pore formation, fusion and fission - often involve time scales of tens of nanometers and milliseconds that are large for atomistic simulation. Frequently, they involve transition states with high curvatures that are difficult to describe by Helfrich-like models. Coarse- grained models can access the relevant time and length scales, allow for a systematic exploration of parameters like the lipid architecture or membrane tension, and they are well suited to study collective phenomena that alter the topology of membranes.

The talk will discuss different computational techniques - Wang-Landau sampling, field-theoretic umbrella sampling, and the string method - to investigate metastable intermediates (like the stalk in the course of membrane fusion) and transition states of pore formation, membrane fusion and fission. Using coarse-grained models, we explore the universal aspects of topology-altering processes in membranes and comment on the extent, to which coarse-grained model capture specific effects of protein-mediated processes.

CPP 43.8 Wed 11:45 H 1028

Formation of Coatless Membrane Vesicles — •Susanne Liese[1], Rossana Rojas[1], Eva Wenzel[2], Camilla Raiborg[2], Harald Stenmark[2], and Andreas Carlson[1] — [1]University of Oslo, Department of Mathematics — [2]Oslo University Hospital, Institute for Cancer Research

The formation of membrane vesicles is an important part of various processes in cell biology. Among others, cells use vesicle formation as an uptake mechanism for controlling their activity and to communicate with other cells through the cargo material that is encapsulated in the membrane vesicle. It all starts with a small initial deformation of the membrane, which subsequently grows and leads to the formation of a vesicle. This dynamic process is induced by membrane associated proteins, which generate forces within the membrane. Membrane compartments inside the cell, such as the endosome, form coatless vesicles but the force generating membrane proteins are not becoming a part of the vesicle. To understand this process, we develop an elastic membrane model to study the biophysical origin of coatless vesicle formation. Our results highlight how elastic membrane parameters and transmembrane proteins determine the shape of the deformed membrane and the equilibrium size distribution of vesicles.

CPP 43.9 Wed 12:00 H 1028

Outperforming nature: synthetic enzyme built from DNA flips lipids of biological membranes at record rates — •Alexander Ohmann[1], Chen-Yu Li[2], Christopher Maffeo[2], Kareem Al Nahas[1], Kevin N. Baumann[1], Kerstin Göpfrich[1], Jejoong Yoo[2], Ulrich F. Keyser[1], and Aleksei Aksimentiev[2] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]University of Illinois at Urbana-Champaign, Champaign, IL, USA

Mimicking enzyme function and increasing performance of naturally evolved proteins is one of the most challenging and intriguing aims of nanoscience. Here, we employ DNA nanotechnology to design a synthetic enzyme that substantially outperforms its biological archetypes. Consisting of only eight strands, our DNA nanostructure spontaneously inserts into biological membranes by forming a toroidal pore that connects the membrane's inner and outer leaflets. The membrane insertion catalyzes spontaneous transport of lipid molecules between the bilayer leaflets, rapidly equilibrating the lipid composition. Through a combination of microscopic simulations and single-molecule experiments we find the lipid transport rate catalyzed by the DNA nanostructure to exceed 10^7 molecules per second, which is three orders of magnitude higher than the rate of lipid transport catalyzed by biological enzymes. Furthermore, we show that our DNA-based enzyme can control the composition of human cell membranes, which opens new avenues for applications of membrane-interacting DNA systems in medicine.

CPP 43.10 Wed 12:15 H 1028

Membrane-mediated interactions between inclusions: the role of shape and background curvature — •Afshin Vahid[1], Andela Saric[2], and Timon Idema[1] — [1]TU Delft, Delft, the Netherlands — [2]University Collage London (UCL), London, United Kingdom

Lipid membranes are vital to cell function. Their combination of fluid and elastic properties allows cells to cope with an out of equilibrium environment. Consequently, membranes exhibit a large variety of shapes, ranging from simple spherical liposomes to complex tubular networks. These shapes are regulated by protein inclusions, that can act both as curvature sensors and curvature inducers. We model the interaction between such inclusions in curved lipid bilayers. We show that in contrast to flat membranes, the inclusions can attract each other and collectively form biologically relevant patterns. For example, we find that even identical inclusions can spontaneously form rings on closed membranes, and those rings again act as curvature sensors. We further demonstrate that the curvature sensing and curvature inducing property of proteins are two sides of the same coin, depending on protein density. In particular, proteins can constrict tubular membranes and facilitate their splitting. This feature was recently observed in mitochondria, and can prevent entanglement with tubes of the ER network also present in the cell.

CPP 43.11 Wed 12:30 H 1028

Membrane curvature and nanobuds generated by lipids with bulky head groups — •Aparna Sreekumari and Reinhard Lipowsky — Theory and Bio-systems, Max Planck Institute of Colloids and Interfaces Golm, D-14424 Potsdam, Germany

We study the mechanical and curvature-elastic properties of bilayer membranes with compositional asymmetry by molecular simulations. The compositional asymmetry is achieved by inserting lipids with a bulky head group into one leaflet (or monolayer) of the bilayer. As we increase the mole fraction ϕ_1 of the bulky-head lipids, we observe a remarkable evolution of the stress profile across the bilayer and a strong increase in the first moment of this profile. In order to extract the spontaneous curvature from this moment, we also determine the bending rigidity of the bilayer which is found to exhibit a non-monotonic dependence on ϕ_1. The latter behaviour reflects changes in the mean density of the lipid tails and head groups. The resulting spontaneous curvature is found to be quite large compared to other molecular mechanisms for bilayer asymmetry. The generated curvature leads to the formation of nanobuds, which provide new membrane compartments, in close analogy to cellular budding processes.

CPP 43.12 Wed 12:45 H 1028

Formation and phase transitions of vapour deposited phospholipid bilayers on porous silicon substrates — Nicolas Moraga[1], Marcelo Cisternas[1], Diego Diaz[1], Rodrigo Catalan[1], Maria J. Retamal[2], Tomas P. Corrales[3], Mark Busch[4], Patrick Huber[4], Marco Soto-Arriaza[2], and •Ulrich G. Volkmann[1] — [1]Institute of Physics and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — [2]Faculty of Chemistry and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — [3]Department of Physics, UTFSM, Valparaiso, Chile — [4]TUHH, Hamburg, Germany

Study of phospholipid artificial membranes on solid substrates has become a relevant way to gain insight into the physical behaviour of cell membranes. In this work, porous silicon substrates (pSi) were made using a two-electrode cell to produce different pore diameters. Substrates were characterized with Field Emission Electron Microscopy. The phospholipid (DPPC) was deposited in high vacuum from the gas phase on the pSi. Film thickness was controlled using Very High Resolution Ellipsometry (VHRE). Samples were hydrated in air with ultrapure water to assemble the bilayer. Phase transitions were measured with VHRE and Stray Light Intensity during temperature cycles. AFM was used to study morphological changes of bilayers as a function of temperature. Our results open new ways to hydrate lipid bilayers using pSi with a specific pore diameter. Acknowledgements: Postdoctoral FONDECYT #3160803 (MJR), FONDECYT #1141105 (UGV) and #1171047 (MSA), FONDECYT INICIACION #11160664 (TPC), CONICYT Fellowships (RC, MC) and CONICYT-PIA ACT 1409.

CPP 44: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials IV (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Wednesday 10:30–13:00 Location: HL 001

Invited Talk CPP 44.1 Wed 10:30 HL 001
Correlating electrons via adiabatic connection approach: a general formalism, approximations, and applications — •Katarzyna Pernal — Institute of Physics, Lodz University of Technology, Poland

Electronic systems are usually described by assuming a model Hamiltonian, which only partially recovers electron correlation effects. To assure a quantitative description one faces a problem of recovering the missing part of the correlation. Over years different methods have been developed, most of them originating from the perturbation theory.

In my talk I will present another, fairly general, approach based on the adiabatic connection formalism. The idea itself is not novel although it has not been considered as a way of adding electron correlation for multireference models. Until recently it has not been realized that by combining the adiabatic connection (AC) with the extended random phase approximation one obtains a general tool capable of accounting for dynamical electron correlation for a broad class of multireference wavefunctions, applicable even to systems including strongly correlated electrons. It will be shown that the AC-based approximation yields excellent results when applied to multireference models, exceeding in accuracy second-order perturbation-theory-based methods.

CPP 44.2 Wed 11:00 HL 001
Density functional theory of electron transfer beyond the Born-Oppenheimer approximation: case study of LiF — •Chen Li[1], Ryan Requist[1], and Eberhard. K. U. Gross[1,2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel

We demonstrate that beyond Born-Oppenheimer (BO) effects can be accurately and seamlessly incorporated within a density functional framework. In alkali halides like LiF, there is an abrupt change in the ground state electronic distribution due to an electron transfer at a critical bond length $R = R_c$. We find that nonadiabatic electron-nuclear coupling produces a sizable elongation of the critical R_c by 0.5 Bohr, an effect which is very accurately captured by a simple and rigorously-derived nuclear mass-dependent correction to the exchange-correlation potential in density functional theory. Since this nonadiabatic term depends on gradients of the nuclear wave function and conditional electronic density, $\nabla_R\chi(R)$ and $\nabla_R n(r, R)$, it couples the Kohn-Sham equations at neighboring R points. Motivated by an observed localization of nonadiabatic effects in nuclear configuration space, we propose an approximation that reduces the search for nonadiabatic density functionals to the search for a single function. This work is a step towards bringing density functional theory beyond the limitations of the BO approximation.

CPP 44.3 Wed 11:15 HL 001
Ground-State Quantum-Electrodynamical Density-Functional Theory — •Michael Ruggenthaler — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

In this talk I present a density-functional reformulation of correlated matter-photon problems subject to general external electromagnetic fields and charge currents [1]. I first show that for static minimally-coupled matter-photon systems an external electromagnetic field is equivalent to an external charge current. I employ this to show that scalar external potentials and transversal external charge currents are in a one-to-one correspondence to the expectation values of the charge density and the vector-potential of the correlated matter-photon ground state. This allows to establish a Maxwell-Kohn-Sham approach, where in conjunction with the usual single-particle Kohn-Sham equations a classical Maxwell equation has to be solved in order to capture the correlation induced by the transversal photon field. In the magnetic mean-field limit this reduces to a current-density-functional theory that does not suffer from non-uniqueness problems and if furthermore the magnetic field is zero recovers standard density-functional theory.

[1] "Ground-State Quantum-Electrodynamical Density-Functional Theory", M. Ruggenthaler, arXiv:1509.01417 (2017).

CPP 44.4 Wed 11:30 HL 001
Design of auxiliary systems for observables: the dynamic structure factor and the electron addition and removal spectra — Marco Vanzini, Martin Panholzer, Lucia Reining, and •Matteo Gatti — LSI, CNRS, Ecole Polytechnique, Palaiseau, France

Density functional theory tells us that the external potential, and therefore all observables, are functionals of the ground state density. The exact functionals, however, are not known, and one has to find approximations. To obtain the density, Kohn and Sham have proposed the idea to use an "auxiliary system". Much research effort goes into finding better and better Kohn Sham potentials for the density and the total ground state energy. In order to access also observables other than the density, we have proposed to generalize the Kohn-Sham idea of an auxiliary system [1], and to design a "connector" that allows us to profit from calculations done in a model system [2,3]. We have recently shown that this is a successful strategy for the dynamic structure factor [2] and for the one-body spectral function of simple metals, semiconductors and insulators [3]. [1] M. Gatti, V. Olevano, L. Reining, and I. V. Tokatly, Phys. Rev. Lett. 99, 057401 (2007) [2] M. Panholzer, M. Gatti, and L. Reining, arXiv:1708.02992 [3] M. Vanzini, L. Reining, and M. Gatti, arXiv:1708.02450

CPP 44.5 Wed 11:45 HL 001
Exact exchange energy of the ferromagnetic electron gas with dipolar interactions — •Camilla Pellegrini, Tristan Mueller, Kay Dewhurst, Sangeeta Sharma, and Eberhard K. U. Gross — Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We propose a density functional treatment of the magnetic dipole-dipole interaction as a spin-spin correction to the Coulomb force in the Breit-Pauli Hamiltonian. Within this microscopic approach, the Hartree-like term for the dipolar coupling corresponds to the classical magnetostatic energy currently implemented in micromagnetic calculations. In addition, we have derived quantum corrections by evaluating analytically the exact exchange energy (Fock term) for the homogeneous electron gas, within the linear response to a noncollinear magnetic field. We expect our functional to open the path towards a full ab initio description of inhomogeneous magnetic structures at the nanoscale, with applications to domain-wall operated spintronic devices.

CPP 44.6 Wed 12:00 HL 001
Precise total-energy calculations at a significantly reduced cost — •Rudolf Zeller — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In density-functional calculations, the total-energy functional is stationary with respect to the density, the Kohn-Sham orbitals and the Kohn-Sham effective potential. This means that approximations for these quantities only lead to total-energy errors of second order provided that the total-energy functional is evaluated accurately without further uncontrolled approximations.

Unfortunately, usually the Kohn-Sham orbitals and thus the kinetic part of the total energy are evaluated by using a projection of the potential into a finite subspace of basis functions. This approximation damages the stationarity of the total energy as a functional of the potential.

A technique will be discussed which can relieve this deficiency so that a considerably smaller subspace of basis functions can be used for a precise evaluation of the kinetic part of the total energy. The advantage will be illustrated for the particular example of angular projection potentials as they are used in the full-potential Korringa-Kohn-Rostoker Green function method.

CPP 44.7 Wed 12:15 HL 001

Approach to Orbital-free DFT with Englert-Schwinger model — •Jouko Lehtomäki and Olga Lopez-Acevedo — COMP Centre of Excellence, Department of Applied Physics, Aalto University, Finland

We briefly present the Englert and Schwinger (ES) model in comparison with other approaches to orbital-free DFT. Essential failure of many kinetic energy density functionals is that they can not describe the most tightly bound core electrons in a satisfactory manner. Englert-Schwinger model allows treating these problematic electrons with more accurate single-particle wavefunctions while still obtaining the self-consistent orbital-free solution to the electronic problem.

Specifically, we detail how the ES model compares to the more known Thomas-Fermi-Dirac-Weizsäcker model self-consistently in atoms. We look at the total energy and few geometric properties. We show qualitative improvement in Pauli potential, which shows unphysical singularities near nucleus when the most tightly bound electrons are not treated correctly. We present how augmentation of the model with Kohn-Sham orbitals allows us to explore all-electron solution to the OFDFT problem and how this paves way for an orbital-free DFT method which does not need pseudopotentials.

CPP 44.8 Wed 12:30 HL 001

The Kerker Preconditioner for FLAPW Methods with Charge Density Mixing — •Miriam Hinzen, Edoardo Di Napoli, Daniel Wortmann, and Stefan Blügel — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In metallic systems of larger size the self-consistent field convergence of electronic structure calculations is often slowed down substantially due to charge sloshing: close to the Fermi level, little change in energy can cause large fluctuations in charge density. Mathematically speaking, the problem is ill-conditioned. For plane-wave methods the Kerker preconditioner effectively solved this problem, but for many other electronic structure methods, in particular all-electron methods as the FLAPW or KKR methods, a real-space formulation would be needed. We developed a formulation of the Kerker preconditioner for FLAPW methods with charge density mixing, implemented in `FLEUR` [1]. Numerical experiments show an enormous reduction of the number of iterations needed for convergence; even more importantly, the SCF convergence has become independent of the system size.
[1] www.flapw.de

CPP 44.9 Wed 12:45 HL 001

Effect of spin on the generalized Pauli constraints in Reduced Density Matrix Functional Theory — •Nicole Helbig[1], Iris Theophilou[2], and Nektarios N. Lathiotakis[3] — [1]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Vass. Constantinou 48, GR-11635 Athens, Greece

Reduced Density Matrix Functional Theory is a method that relies on the 1-1 correspondence between the many-body ground-state wave function and the first order reduced density matrix (1RDM) and uses the latter as its fundamental variable. Enforcing the generalized Pauli constraints during the energy minimization ensures that the 1RDM corresponds to a fermionic pure state. We demonstrate that these constraints are modified for open-shell systems if the spin degrees of freedom are taken into account. From the generalized Pauli constraints we also derive properties of the exact occupation numbers and natural orbitals which ensure that the 1RDM corresponds to an eigenstate of the total spin.

CPP 45: Charged Soft Matter, Polyelectrolytes and Ionic Liquids I

Time: Wednesday 11:00–13:00 Location: C 243

Invited Talk CPP 45.1 Wed 11:00 C 243

Double-Semidilute Liquid and Gel Coacervates formed by Oppositely Charged Polyelectrolytes — •Michael Rubinstein[1], Sergey Panyukov[2], and Qi Liao[3] — [1]Duke University, Durham, NC, USA — [2]P. N. Lebedev Physics Institute, Moscow, Russian Federation — [3]Chinese Academy of Sciences, Beijing, China

We develop a scaling model for two qualitatively different classes of coacervates formed by oppositely charged polyelectrolytes. The weakly interacting coacervates are liquids with electrostatic interaction energy per charge less than thermal energy kT. The strongly interacting coacervates are gels with cross-links formed by ion pairs of opposite charges attracting each other with energy stronger than kT. The liquid coacervate is a double-semidilute solution with two correlation lengths and two qualitatively different types of conformations of weaker and stronger charged polyelectrolytes. Weaker charged chains form a screening "coat" around stronger charged chains. The conformations of weaker charged chains in this screening coat is analogous to a semidilute solution of uncharged polymers. The conformation of stronger charged polyelectrolytes in liquid coacervates is similar to their conformation in semidilute polyelectrolyte solutions. The strongly interacting coacervates form bottlebrush gels for longer polyelectrolytes with higher charge density and star-like gels for shorter higher charge density chains.

CPP 45.2 Wed 11:30 C 243

Dendritic polyelectrolytes and their interaction with proteins: Simulation perspective — •Rohit Nikam[1,2], Xiao Xu[1,2], Qidi Ran[1], Matej Kanduč[1], Rainer Haag[3], Matthias Ballauff[1], and Joachim Dzubiella[1,2] — [1]Institut für Weiche Materie und Funktionale Materialien, Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [3]Multifunctional Biomaterials for Medicine, Helmholtz Virtual Institute, Kantstr. 55, 14513 Teltow-Seehof, Germany

Dendritic polyelectrolytes constitute high potential drugs and carrier systems for biomedical purposes, yet their interaction modes with biomolecules have not been microscopically characterized. We investigate key electrostatic, hydration and structural features of dendritic polyglycerol sulfate (dPGS) and its interaction with biologically important serum proteins using molecular simulations complemented by isothermal titration calorimetry (ITC) and electrophoretic measurements. We demonstrate that the driving force for the strong complexation originates mainly from the release of only a few condensed counterions from dPGS upon binding. The binding constant shows surprisingly weak dependence on dPGS size (and bare charge) which can be explained by charge-renormalization effects and by the fact that the magnitude of the dominating counterion release mechanism is sensitive exclusively to the interfacial charge structure of the protein-specific binding patch. Our results open new perspectives for the rational design of charged polymeric drugs and carrier systems.

CPP 45.3 Wed 11:45 C 243

The effect of weakly and strongly interacting cations on phase behaviour of protein solutions — •Olga Matsarskaia[1], Felix Roosen-Runge[2], Gudrun Lotze[3], Johannes Möller[3], Fajun Zhang[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]Division of Physical Chemistry, Lund University, Lund, Sweden — [3]ESRF, Grenoble, France

Multivalent cations can induce a rich phase behaviour including reentrant condensation, clustering, liquid-liquid phase separation with a lower critical solution temperature (LCST-LLPS) and crystallisation [1], [2] in aqueous protein solutions. Interestingly, these phase behaviours strongly depend on cation-specific properties. Comparing different rare-earth metals, we find a strong decrease of an LCST-related transition temperature (T_{trans}) with decreasing cation radius. This result is complemented by a thermodynamic characterisation of cation-protein binding revealing a decrease in the point of zero charge for smaller cations. Finally, significant differences in cation-induced protein-protein interaction strengths are observed using small-angle x-ray scattering (SAXS). Importantly, these point towards the fact that in addition to their radius, other cation-specific effects such as polarisability and orbital occupation can play a crucial role in cation-protein interactions. Our findings thus indicate that a careful choice of a suitable multivalent salt can help tailor protein phase behaviour [3].

[1] Zhang *et al.* Pure & Appl. Chem. 2014, 86, 191-202; [2] Matsarskaia *et al.* JPCB 2016, 120, 7731-7736; [3] Matsarskaia *et al. in preparation.*

CPP 45.4 Wed 12:00 C 243

Effects of anions on the reentrant phase behavior in protein solutions induced by multivalent salts — •Michal K. Braun[1], Andrea Sauter[1], Simon Schoenberg[1], Michael Sztucki[2], Fajun Zhang[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ESRF, Grenoble, France

Interactions between ions and proteins are a highly active research field. They are important both in metabolic processes and to more generally understand protein phase behavior [1]. Model globular proteins in solution with trivalent salts exhibit a reentrant phase behavior where in the condensed regime the cation serves as a linker between two proteins [2, 3]. The nature of the condensates is tunable by the specific cations and anions that are employed. The microscopic role of the anion is not yet fully understood. However, it has now been observed that NO_3^- salts lead to a stronger attraction compared to Cl^- salts. This result is consistently obtained by visual inspection of the sample solutions, by monitoring the protein concentration in the supernatant using UV-vis absorption spectroscopy and by extracting potential parameters from model fits to small angle x-ray scattering data. This suggests a different affinity of Cl^- vs. NO_3^- to the protein surface. Possible microscopic reasons such as Hofmeister effects and different entropy contributions of the anions will be discussed.

[1] Gunton et al., *Protein Condensation*, 2007 [2] Zhang et al., *Pure Appl. Chem.*, **86**, 191, 2014 [3] Matsarskaia et al., *J. Phys. Chem. B*, **120**, 7731, 2016

CPP 45.5 Wed 12:15 C 243

The influence of co-solutes on the chemical equilibrium - a Kirkwood-Buff theory for ion pair formation processes in ternary solutions — •anand narayanan krishnamoorthy, christian holm, and jens smiatek — Institute for Computational Physics - University of Stuttgart

We present a theoretical framework for ternary solutions in order to describe the influence of co-solute species on the chemical equilibrium of ion pair formation. The theory relies on the use of Kirkwood-Buff integrals and the introduction of a local/bulk partition model. We can show that either ion pair formation or ion dissociation is favored with regard to a more pronounced co-solute accumulation around the corresponding ion state. The co-solute molecules can be either charged or uncharged and the theory is applicable for ideal and weakly nonideal solutions in combination with low ion concentrations. The corresponding implications of our theory are useful in order to optimize the efficiency of electrolyte solutions in electrochemical applications. All theoretical results are verified by atomistic molecular dynamics simulations of sodium chloride ion pairs in dimethylacetamide (DMAc)/water mixtures.

CPP 45.6 Wed 12:30 C 243

Binary mixtures of ionic liquids and co-solutes: the local structure at uncharged walls in presence of dimethyl sulfoxide and water — Takeshi Kobayashi[1], Maria Fyta[1], and •Jens Smiatek[1,2] — [1]University of Stuttgart, Institute for Computational Physics, D-70569 Stuttgart, Germany — [2]Helmholtz Institute Münster (IEK-12 HI MS), Forschungszentrum Jülich, D-48149 Münster, Germany

We study the local structure of binary ionic liquid mixtures, namely 1-ethyl-3-methylimidazolium dicyanamide (EMIM/DCA) in combination with varying mole fractions of co-solutes dimethyl sulfoxide (DMSO) and water in front of uncharged and purely repulsive walls. In agreement with recent experimental results [1], we observe significant differences in our atomistic molecular dynamics simulations between the local accumulation behavior of the co-solutes at the interfaces. The corresponding bulk solvation structure provides more insights into these effects, which can be attributed to non-idealities in the local distribution of the molecules. Our recently introduced Kirkwood-Buff approach for ionic liquids [2] helps us to shed more light on the corresponding findings.

[1] M. Jitvisate et al., J. Phys. Chem. C 121, 18593 (2017)
[2] T. Kobayashi et al., Phys. Chem. Chem. Phys. 19, 18924 (2017)

CPP 45.7 Wed 12:45 C 243

Competing interactions and the formation of dynamic protein clusters — •Anita Girelli[1], Michal K. Braun[1], Felix Roosen-Runge[2], Marco Grimaldo[3], Tilo Seydel[3], Fajun Zhang[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]Physical Chemistry, Lund University, Sweden — [3]ILL Grenoble, France

Protein clusters are potential precursors for protein crystallization. The question of their formation and transient, dynamic or permanent nature is of high relevance to structural biology and biomedicine. Here we report on protein clusters in bovine serum albumin (BSA) - trivalent salt (YCl_3, $LaCl_3$) systems. The protein clusters are most probably held together by ion bridges and precede a condensation regime [1, 2]. The clusters are characterized by dynamic light scattering (DLS). For a molar ratio of salt concentration and protein concentration, c_s/c_p, equal to 4, we can observe the formation of clusters with a lifetime longer than 1 ms. Based on a comparison with self-diffusion data from neutron back scattering experiments [3], we assume that dynamic clusters form for c_s/c_p between 2 and 4. Furthermore, SAXS measurements for samples under these conditions demonstrate the competing interactions, which support the formation of dynamic clusters.

[1] Soraruf et al., *Soft Matter*, **10**, 894, 2014
[2] Zhang et al., *J. Appl. Cryst.*, **44**, 755, 2011
[3] Grimaldo et al., *J. Phys. Chem. Lett.*, **6**, 2577, 2015

CPP 46: Poster Session IV

Topics: Fundamental Physics of Perovskites (46.1-46.7), Hybrid and Perovskite Photovoltaics (46.8-46.21), Organic Electronics and Photovoltaics (46.22-46.47), Molecular Electronics and Photonics (46.48-46.51), Excitons, Plasmons and Polaritons in Molecular Systems (46.52-46.53), Electrical, Dielectrical and Optical Properties of Thin Films (46.54-46.58).

Time: Wednesday 11:00–13:00 Location: Poster A

CPP 46.1 Wed 11:00 Poster A

Control of Charge-Carrier Concentration in Lead-Free Perovskite Thin Films Consisting of Formamidinium Tin Iodide — •Pascal Schweitzer, Jonas Horn, Raffael Ruess, and Derck Schlettwein — IAP, JLU Giessen, Germany

As a promising substitute material for toxic lead perovskites we investigated formamidinium tin iodide. Thin films were prepared by spin-coating in a one-step approach. The crystal structure was confirmed by XRD, the microstructure of the films was studied by SEM and the optical absorption characteristics (Burstein-Moss-shift) were investigated by UV-vis spectroscopy. To discuss optoelectronic applications of such films, understanding of the electronic characteristics is essential. Different measurement geometries and contact materials were tested in order to provide reliable electrical studies. Inert contact materials and symmetrical electrodes were used to concentrate on perovskite materials properties rather than the influence of additional hole- and electron transport layers in typical device structure. To avoid severely high charge carrier concentrations caused by self-doping, this was limited by intentional mixing with tin fluoride to compensate tin vacancies. Current-voltage-characteristics served to discuss hysteresis in the materials which led to insight into polarization effects that are crucial, e.g. for perovskite solar cells under working conditions. We applied impedance spectroscopy to Schottky-type contacts to follow the space charge capacity under potential variation. Thereby we determined the charge carrier concentration in dependence of permittivity via Mott-Schottky analysis.

CPP 46.2 Wed 11:00 Poster A

Charge Injection from $CH_3NH_3PbI_{3-x}Cl_x$ to Organic Semiconductors Detected With sub-ps Transient Absorption Spectroscopy — •Jonas Horn[1], Iulia Minda[2], Heinrich Schwoerer[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, JLU Giessen, Germany — [2]Laser Research Institute, Stellenbosch University, South Africa

Presently, inverted perovskite solar cells are heavily studied. The charge transfer processes between the perovskite layer and the charge extraction layers is one of the key factors in solar cell performance. In most of these architectures, a combination of PEDOT:PSS as transparent hole conductor and PCBM as n-type semiconductor is used. In this study, pump-probe absorption spectroscopy with femtosecond resolution is used to determine the injection time of photo-generated charge carriers from the perovskite to the PEDOT:PSS and PCBM layers. A characteristic signal was identified to be caused by holes injected into the PEDOT:PSS layer by comparing the transient signals of photo-excited perovskite films with and without PEDOT:PSS interface. This signal appears within the resolution of the measurement setup (<200 fs) proving ultrafast charge carrier injection. Changes in the transient signals characteristic for the perovskite layer as reflected in the time constants obtained by global analysis confirmed this observation. We could also show ultrafast as well as slow injection of electrons into PCBM based on the decay of signals characteristic for the excited state of the perovskite as well as the appearance of characteristic PCBM signals.

CPP 46.3 Wed 11:00 Poster A

In-situ monitoring of sequential conversion of MAPb(IxBr1-x)3 — •Carolin Rehermann, Katrin Hirselandt, Aboma Merdasa, and Eva Unger — Helmholtz-Zentrum Berlin, Young Investigator Group Hybrid Materials Formation and Scaling, Berlin, 12489, Germany

Metal halide perovskites are an interesting material for tandem solar cells due to their band gap tunability, band gaps up to 3 eV can be prepared by exchanging halides.1 Burschka et al.2 introduced the 2-step method. Three competing processes might occur: direct conversion/intercalation, dissolution-reformation and ion exchange.3

In this work, the second step is monitored by in-situ UV-vis measurements. The second step is the conversion from a lead iodide film into a mixed halide perovskite film MAPb(IxBr1-x)3. Using MABr we can track the different conversion kinetics between a direct conversion and a dissolution-reformation process. The influence of different reaction parameters is investigated.

In-situ UV-vis measurements show an initial evolution of a spectral signature characteristic for the absorption onset of the direct conversion product, MAPbBrI2. Upon progression, this signature disappears in favor of the pure dissolution-reformation product MAPbBr3. Changes in spectral signature during a post-conversion annealing step prove that ionic equilibration occurs.

1. Unger et al. Journal of Materials Chemistry A 2017, 5 (23), 11401-11409. 2. Burschka et al. Nature 2013, 499 (7458), 316-319. 3. Ko et al. Chemistry of Materials 2017, 29 (3), 1165-1174.

CPP 46.4 Wed 11:00 Poster A

Combinatorial Investigation of Co-Evaporated $CsPbI_3$ Thin Films — •Pascal Becker, Justus Just, and Thomas Unold — Helmholtz-Zentrum Berlin, Germany

Lead halide Perovskite materials have recently emerged as very promising new material for thin film solar cell absorbers yielding power conversion efficiencies of above 22 %. Highest power conversion efficiencies are found for Pb-based inorganic-organic halides, which tend to chemically decompose at elevated temperatures. Inorganic lead halide perovskites such as $CsPbI_3$ are significantly more stable and well suited candidates for high efficient tandem solar cells due to their high bandgap of 1.8 eV. However, much less is known about the crystal structure and optoelectronic properties of these compounds.

We synthesized combinatorial samples of $CsPbI_3$ thin films with a spatial gradient in composition by co-evaporation of CsI and PbI_2. Applying X-ray diffraction mapping, X-ray fluorescence mapping and UV-vis mapping on these samples we are able to investigate the phase diagram of this compound as well as the optoelectronic properties of the different phases. Depending on the composition and growth temperature we find a transition from the yellow phase to the brown phase in $CsPbI_3$ as well as segregation of excess CsI and PbI_2.

CPP 46.5 Wed 11:00 Poster A

In-Situ Investigation of Ion Migration and Aggregation in Organolead Halide Perovskite Films — •Yu Zhong[1], Carlos Andres Melo Luna[2], Richard Hildner[2], Cheng Li[1], and Sven Huettner[1] — [1]Macromolecular Chemistry I, University of Bayreuth, Bayreuth, Germany — [2]Experimental Phyiscs IV, University of Bayreuth, Bayreuth, Germany

During current-voltage(J-V) measurements, perovskite solar cells(PSCs) exhibit a certain photo-induced instability and hysteresis phenomenon. Firstly, we study the light-induced behavior in CH3NH3PbI3-xClx film in-situ, by employing wide-field photoluminescence(PL) microscopy to obtain both the spatially- and temporally-resolved PL image. Along with the increase of the PL intensity under continuous illumination, some areas render PL inactive. A faster and more obvious PL decay process was observed with a higher excitation energy. By characterizing this excitation energy dependent PL decay, we suggest that the PL quenching can be ascribed to an aggregation of iodide ions. Secondly, by introducing phenyl-C61-butyric acid methyl ester(PCBM) in PSCs, hysteresis phenomenon is suppressed. The results of wide-field PL image and temperature dependent J-V curve measurement confirm that PCBM molecules decrease the mobility and increase the activation energy of iodide ions. This real-time investigation of the light soaking of perovskite films provides more details to improve the performance of PSCs. The suppression of the iodide ions movement, e.g. involving PCBM, is a concern for better performance and stability of PSCs.

CPP 46.6 Wed 11:00 Poster A

Influence of hole selective contacts in inverted perovskite solar cells — •Katrin Hirselandt[1], Aniela Czudek[1], Celline Awino[2], Steffen Braunger[1], Carolin Rehermann[1], Thomas Dittrich[2], and Eva Unger[1] — [1]Helmholtz-Zentrum Berlin, Young Investigator Group Hybrid Materials Formation and Scaling, Berlin, 12489, Germany — [2]Helmholtz-Zentrum Berlin, Institute Silicon Photovoltaics, Berlin, 12489 Berlin, Germany

Planar solution processed perovskite solar cells have reached efficiencies above 20 % and their stability have improved during the past years [1,2]. In device preparation, reproducibility is a major obstacle due to perovskite absorber inhomogeneity and interfacial properties [3].

In this study we investigated four different types of planar inverted perovskite solar cells, comparting the cesium-containing triple cation perovskite with the archeotypical methylammonium lead iodide (MAPI) as absorber materials as well as two different hole transporting materials (HTMs): Poly[bis(4-phenyl)(2,4,6-trimethylphenyl)amine] (PTAA) and Poly(3,4-ethylendioxxythiophene) polystyrene (PEDOT:PSS) as selective contact layer.

The best and most reproducible performance of 16 % on average was achieved for MAFACs on PTAA. These devices also exhibited the least photocurrent hysteresis and are hence the most robust and reproducible architecture tested.

[1] K. A. Bush et al., Nature Energy (2017), 2, 17009 [2] M. A. Green et al., Prog. Photovoltaics (2017), 25, 3-13 [3] C. Bi et al., Nature Communications (2015), 6, 7747

CPP 46.7 Wed 11:00 Poster A

Measurement development for hysteresis characterization of perovskite solar cells — •Aniela Czudek[1], Lukas Kegelmann[1], Amran Al-Ashouri[1], Steve Albrecht[1], and Eva Unger[1,2] — [1]Helmholtz-Zentrum Berlin fur Materialien und Energie, Berlin, Germany — [2]Lund University, Department of Chemical Physics, Lund, Sweden

Evaluating the performance of perovskite solar cells can be intricate due to transient current-voltage phenomena on different time scales. Current-voltage measurements in different scan directions may exhibit varying degrees of discrepancy - often referred to as hysteresis - which makes defining the 'right' measurement conditions difficult. We here present a procedure to assess the steady-state solar cell performance of perovskite devices using an iterative - perturb and observe - maximum power point tracking algorithm. This methodology is directly used to also investigate the transient response of devices upon voltage perturbation around maximum power point. The time constants of transient current response allows for a quantitative comparison of different device architecture types and determine the minimum delay time (voltage settling time) required to perform current-voltage measurements at quasi-steady-state condition of the device. We will show and discuss how this methodology was utilize to quantitatively compare perovskite solar cells of different architecture types, contact layers and perovskite absorber composition.

CPP 46.8 Wed 11:00 Poster A

Investigation of inorganic nanoparticles and low band-gap polymers for printed hybrid solar cells — •Gaetano Mangiapia and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Printed solar cells represent a potential alternative to the use of conventional cells. Because of their low-cost, low-weight, production simplicity, and possibility to be used on curved or flexible substrates, they have progressively captured the attention of applied research. Printed hybrid solar cells combine the above mentioned advantages with the use of hybrid photovoltaics, where two different semiconductors (organic and inorganic) compose the active layer. Although PCE values need to be boosted up for industrial applications, the possibility to chemically modulate the properties of the organic part (e.g. by adding or changing a functional group) allowed foreseeing the capability to tune both the optical and electronic properties, an essential requirement for finding new and highly efficient materials. We study bulk heterojunction hybrid solar cells composed of the low band-gap polymer PTB7 and its derivatives and inorganic ZnO nanoparticles. We correlate optical and morphological properties of the active layer. Characterization involves X-ray and neutron scattering techniques in combination with photophysical measurements.

CPP 46.9 Wed 11:00 Poster A

Hybrid solar cells based on metal oxides and water-soluble polythiophenes — •Jiabin Gui[1], Volker Körstgens[1], Klara Stallhofer[2], Hristo Iglev[2], Reinhard Kienberger[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]TU München, Physik-Department, LS Laser und Röntgenphysik, 85748 Garching

Environmentally friendly processing of hybrid solar cells with the solvent water is feasible with an active layer consisting of laser-ablated metal oxides and a water-soluble polythiophene [1]. Zinc oxide and titanium dioxide particles are processed with laser ablation in water. The obtained nanoparticles are investigated regarding the size distribution and crystallinity. Spray-deposition as a cost-effective preparation method has been utilized as technique to produce films of the laser-ablated nanoparticles, the active layers including polythiophenes and the corresponding hybrid solar cells. Films have been characterized with optical and spectroscopic methods as well as with x-ray characterization techniques. The influence of differences of bandgap, crystallinity and mesoscale morphology on the photovoltaic performance of the obtained devices is discussed. [1] Körstgens et al., Nanoscale 7, 2900 (2015).

CPP 46.10 Wed 11:00 Poster A

Use of Triphenylamine Dyes With Metal Complex Electrolytes in ZnO-Based Dye-Sensitized Solar Cells . — •Andreas Ringleb, Raffael Ruess, and Derck Schlettwein — IAP, JLU Giessen, Germany

Dye-sensitized solar cells (DSSCs) may serve as an alternative to silicon-based solar cells because of low energy-payback-times and expected low costs, in particular, if the porous ZnO is prepared by electrodeposition. The triphenylamine-based organic dye D35CPDT (also known as LEG4) has been frequently used as a sensitizer with good efficiency on TiO_2 in combination with modern Co- and Cu-based electrolytes which have a high redox potential and allow fast and effective regeneration without high overpotentials. In the present work we study the combination of these different successful approaches. Porous ZnO has been electrodeposited on AZO-coated glass. Adsorption of LEG4 to the ZnO surface has been studied by varying pre-treatment of the films and optimized samples have been used to prepare DSSCs. These have been studied by means of current-voltage characteristics and detailed photoelectrochemical methods such as impedance spectroscopy, dynamic illumination and time-resolved experiments. A focus has been put on the analysis of recombination of injected electrons from the ZnO/dye interface to the redox electrolyte as one of the main loss channels in DSSCs and on mass transport of the electrolyte through the porous sensitized photo anode as an additional limiting factor.

CPP 46.11 Wed 11:00 Poster A

Control of surface electronic parameters of ITO using dipolar monomolecular layers. — •Meysam Raoufi[1], Ulrich Hörmann[1], Emil list Kratochvil[2], and Dieter Neher[1] — [1]University of Potsdam, Institute of Physics and Astronomy, Potsdam-Golm, Germany — [2]Humboldt University, Institute for Physics, Berlin, Germany

In organic electronic devices, the injection of holes and electrons from the electrodes into the organic semiconductors is a key issue for their efficient operation. Different chemical and physical treatments have been proposed to improve hole injection and minimize the injection barrier height as a result of increasing the work function of ITO. A particularly interesting approach is the deposition of dipole layers by molecular self-assembly[1,2].

Here, by applying self assembled monolayers of different phosphonic acids, we study how the efficiency of hole injection across a hybrid surface correlates with the change in barrier height. Fine tuning of the injection barrier is achieved by mixing molecules with different electrostatic dipoles. Finally, by incorporating photo-switchable molecules into the SAM, we gain control over the energetics at the organic/inorganic interface and its injection properties.

1. A. Sharma, A. Haldi, P. J. Hotchkiss, S. R. Marder, and B. Kippelen, J. Appl. Phys. 105, (2009). 2. I. Lange, S. Reiter, M. Pätzel, A. Zykov, A. Nefedov, J. Hildebrandt, S. Hecht, S. Kowarik, C. Wöll, G. Heimel, and D. Neher, Adv. Funct. Mater. 24, 7014 (2014).

CPP 46.12 Wed 11:00 Poster A

Work-Function Modification of Transparent Conductive Electrodes and Investigation of Organic Electron-Transport-Layers for Use in Perovskite Solar Cells — •Berthold Wegner[1,2], Federico Pulvirenti[3], Jay Patel[4], Nakita Noel[4], Henry Snaith[4], Seth Marder[3], and Norbert Koch[1,2] — [1]Helmholtz-Zentrum Berlin, Germany — [2]Humboldt-Universität zu Berlin, Germany — [3]Georgia Institute of Technology, Atlanta, USA — [4]University of Oxford, UK

Minimizing electron-collection losses at the electron-selective contact in organic-inorganic halide perovskite solar cells is crucial to achieve better device performance and long-term stability. Here, we report on the modification of fluorinated tin oxide (FTO) used as transparent electrode in perovskite devices, and the comparison of two classes of organic semiconductors with similar electron affinities for their use as efficient electron-transport-layers (ETL) in perovskite solar cells. Ultraviolet photoelectron spectroscopy (UPS) reveals that deposition of a moderately air-stable organometallic dimer on the FTO surface leads to a decrease in work-function (WF) by more than 1 eV. Furthermore, UPS and x-ray photoelectron spectroscopy (XPS) are used to study the energy level alignment between the dimer-modified FTO and the ETL layers, and whether the dimer reacts with or diffuses into the ETL layer. Perovskite solar cells employing such modified electron-selective contacts were fabricated showing increased power conversion efficiencies.

CPP 46.13 Wed 11:00 Poster A

Suppressed Ionic Migration in 2D-Ruddlesden-Popper Perovskite — •Cheng Li[1], Antonio Guerrero[2], Huan Long[1], Yu Zhong[1], Juan Bisquert[2], Jianpu Wang[3], and Sven Huettner[1] — [1]Organic and Hybrid Electronics, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany — [2]Institute of Advanced Materials (INAM), Universitat Jaume I, 12006 Castellö, Spain — [3]Institute of Advanced Materials (IAM), Nanjing Tech University (NanjingTech), 30 South Puzhu Road, Nanjing 211816, China

Organometal trihalide perovskite solar cells (PSCs) are still suffering from the problem of hysteresis and stability. Recently, another class of perovskite - two dimensional (2D) Ruddlesden-Popper (RP) halide layered perovskites have attracted attention. In this work, first, we fabricate 2D RP perovskites using 1-naphthylmethylamine iodide (NMAI) as the precursor. Then we characterize the built-in potential in the device using electroabsorption spectroscopy. Further, we utilize time-resolved photoluminescence (PL) image microscopy and impedance spectroscopy (IS) on perovskite films to investigate both the spatial and temporal evolution of ion migration under external electric fields. Our approach enables us to quantitatively characterize the kinetic processes and determine the mobility of these ions, which is around one order of magnitude lower compared with the one in 3D perovskite. Following that, temperature dependent J-V curve enables us to obtain the activation energy of ions inside. Hence, decrease of J-V curve hysteresis and the improvement on stability are ascribed to the suppressed ion migration.

CPP 46.14 Wed 11:00 Poster A

Radiative efficiency in planar metal-organic-perovskite solar cells — •Simon Berger[1], Philipp Rieder[1], David Kiermasch[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), 97074 Würzburg

In order to achieve an ideal solar cell with any material system, it is necessary to strive for the radiative efficiency limit. Here we evaluated the capability of planar perovskite solar cells in (p-i-n)-layout to emit light by EL-spectroscopy. In this technique charge carriers are injected into the solar cell to recombine and the emitted photons are being detected. We fabricated and evaluate devices with different hole transport layers namely PTAA, PEDOT-PSS and p-TPD. The $MAPbI_3$ and $(MAPbBr_3)_x(FAPbI_3)_{(1-x)}$ perovskites were prepared by both the one-step and two-step method. We show the impact of these different charge selective layers and the applied voltage on the electro-luminescence characteristics and compute $V_{OC,Rad}$ in the radiative limit for each material.

CPP 46.15 Wed 11:00 Poster A

Charge Carrier Dynamics in Methylammonium Lead Iodide probed by TRMC and TRPL — •Nathania Henning[1], Manuel Ullrich[1], Liudmila Kudriashova[1], Andreas Baumann[2], Andreas Sperlich[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Organo lead halide perovskites, such as methylammonium lead iodide (MAPI), have attracted great attention to the field of thin film photovoltaics due to their outstanding electrical and optical properties. The mobility and the lifetime of photogenerated charge carriers are among the fundamental quantities which define the performance of solar cell devices. In this work, we perform combined analysis of transients, provided by two electodeless characterisation techniques: time-resolved microwave conductivity (TRMC) and time-resolved photoluminescence (TRPL). Complementary TRMC and TRPL characterisation of perovskite thin films aims to improve numerical fits and provide characteristic lifetimes as global fit parameters.

CPP 46.16 Wed 11:00 Poster A

Time-Resolved Microwave Conductivity on Perovskite Materials for Solar Cells — •Manuel Ullrich[1], Nathania Henning[1], Liudmila Kudriashova[1], Andreas Baumann[2], Andreas Sperlich[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Perovskite solar cells have attracted much attention in recent years, since their power conversion efficiencies increased steadily and exceeded 20 %. To further improve their performance and relate this to the preparation route, optoelectronic properties need to be investigated. We use time-resolved microwave conductivity (TRMC) to elucidate and quantify charge carrier mobilities and lifetimes. This electrodeless technique is based on the interaction of photoexcited charge carriers with the applied electro-magnetic field (GHz), leading to a time-dependent change in conductance. We focus on methylammonium lead iodide ($CH_3NH_3PbI_3$) as an active layer and examine different processing conditions, which affect the perovskite crystallinity and finally the charge carrier dynamics. Furthermore the impact of different transport layers on the charge carrier lifetime is investigated.

CPP 46.17 Wed 11:00 Poster A

Characterization of mm sized $CH_3NH_3PbI_3$ crystals grown by Inverse Temperature Crystallization — •Stefan Kiesmüller[1], Stefan Väth[1], Sebastian Hammer[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

Organo lead halide perovskites are an important subject of research due to their promising properties concerning photovoltaics. Up to now, mostly thin films with poly-crystalline nature are formed from solution or vacuum deposition techniques. The role of crystallinity and crystal domain size on the functionality of the perovskite solar cell is in the focus of present research. In order to probe the fundamental properties like the charge carrier transport of the hybrid perovskite semiconductors and its limitations very often large crystals have been studied. Here, we used the technique of Inverse Temperature Crystallisation to grow methylammonium lead iodide (MAPI) crystals of different size and crystal quality. This growth technique for crystals is based on the effect of reverse solubility of some materials in special solvents in remarkably short growth times. The so grown MAPI crystals are characterized by means of X-ray diffraction and scanning electron microscopy. The optical properties are studied by photoluminescence. Finally, Time-of-Flight measurements were performed to investigate the fundamental charge carrier transport.

CPP 46.18 Wed 11:00 Poster A

$Cs_2AgBiBr_xI_{1-x}$: A Novel Lead-Free Material for Perovskite Solar Cells — •Melina Armer[1], Mathias Fischer[1], Liudmila Kudriashova[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

As conventional perovskite solar cells contain lead and therefore suffer toxicity issues, finding alternative lead-free materials for the application in perovskite photovoltaics has become an essential problem to be solved. In this work, we present a novel lead-free material for solar cells, $Cs_2AgBiBr_xI_{1-x}$, permitting straightforward spin-coating from solution. The films have been characterized using steady state and time-resolved optical spectroscopy. The morphology and quality of the as prepared films has been evaluated using a scanning electron microscope and X-ray Diffraction. It has been found that solution processed $Cs_2AgBiBr_xI_{1-x}$ forms polycrystalline thin films with crystalline domains in the micrometer range. Further, we observed photoluminescence in the visible region (around 658 nm) with long lifetimes up to 1,6 μs in the visible region by steady state and time resolved photoluminescence measurements. Due to the encouraging optical properties, the straightforward solution processing and its uniform polycrystalline morphology we propose $Cs_2AgBiBr_xI_{1-x}$ to be a promising candidate for the application in lead-free perovskite solar cells.

CPP 46.19 Wed 11:00 Poster A

Rotational dynamics of methyl ammonium ions in the hybrid organic-inorganic perovskite $CH_3NH_3PbI_{2.94}Cl_{0.06}$ by means of QENS investigations — •Götz Schuck[1], Frederike Lehmann[1,2], and Susan Schorr[1,3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Universität Potsdam, Institut für Chemie, Potsdam OT Golm, Germany — [3]Institute of Geological Sciences, Freie Universität Berlin, Berlin, Germany

Perovskites with ABX_3 - structure show a huge possibility on element substitutions on A-, B- and X-site which leads to a broad variety of physical properties. Our main field of interest is chloride substituted methyl ammonium lead triiodide in which A is the organic unit $[CH_3NH_3]^+$ = MA, B = Pb_2^+ and X = $I_{3-x}Cl_x$. The aim is to get an inside into the interrelationship of static and dynamic structure of $MAPbI_{3-x}Cl_x$ and $MAPbCl_3$ by studying the temperature dependent methyl ammonium dynamics by means of QENS investigations in order to understand the influence of chloride on the rotational dynamics of the methyl ammonium cation.

In recent QENS investigations on $MAPbI_3$ [1] two quasielastic components were identified in the tetragonal (165 K < T < 327 K) and cubic (T > 327 K) phase. From the QENS results, it was interpreted that in the cubic and tetragonal phases the MA ion exhibit four-fold rotational symmetry perpendicular to the C-N axis (C_4) along with three-fold rotation parallel to the C-N axis (C_3), while in the orthorhombic *Pnma* phase (T < 165 K) only C_3 rotation is present.

[1] Li et al., Nature Communications 2017, 8, 16086

CPP 46.20 Wed 11:00 Poster A

Charge carrier recombination in planar n-i-p and p-i-n perovskite solar cells - the role of interfaces — •D. Kiermasch[1], K. Tvingstedt[1], L. Gil-Escirg[2], C. Momblona[2], M. Sessolo[2], A. Baumann[3], H. Bolink[2], and V. Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg, Germany — [2]Instituto de Ciencia Molecular, Universidad de Valencia, 46980 Paterna, Valencia, Spain — [3]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg, Germany

Charge carrier recombination processes in organo-metal halide perovskite solar cells are one of the most studied research topics in this new class of photovoltaic materials. Usually, time resolved photoluminescence (tr-PL) is used to study recombination in perovskite layers. Here, crystals or films with or without charge selective layers are being probed. In contrast, only a few experimental approaches have been presented on complete perovskite solar cells using charge selective layers and contacts.

We report on charge carrier recombination dynamics in planar n-i-p and p-i-n perovskite solar cells with different organic charge selective layers. The perovskite layers have been prepared by vacuum deposition leading to efficiencies in the range of 20% for the n-i-p and 17% for the p-i-n layout. To explain this difference between both type of devices we studied charge carrier recombination dynamics with steady state and transient electrical measurements demonstrating the importance of interface recombination in perovskite solar cells.

CPP 46.21 Wed 11:00 Poster A

Red-shifting the band gap of Perovskite photovoltaics using Sn/Pb metal mixtures — •Antonio Günzler and Michael Saliba — Adolphe Merkle Institute, Fribourg, Switzerland

Perovskite solar cells using only Pb at the metal position currently achieve record performances. Partial replacement of Pb by Sn has the advantage of using less toxic Pb.

In addition, Pb-Sn mixtures have an earlier absorption onset towards the near IR broadening the absorption spectrum. This is especially useful for thin-film perovskite-perovskite tandem cells already achieving up to 19% efficiency to date with the potential to reach values beyond 40%.

Furthermore, other optoelectronic applications require tunability of the band gap.

We aim to improve the fundamental understanding of the correlation between the perovskite structure and its optoelectronic properties under variation of the Sn content.

CPP 46.22 Wed 11:00 Poster A

Interfacial charge transfer and temperature dependent charge carrier transport in organic heterostructure field-effect transistors — •Eduard Meister, Stefan Schmidt, and Wolfgang Brütting — Institute of Physics, University of Augsburg, Germany

In this work we studied interfacial charge transfer (CT) happening in hetero-structure field-affect transistors (FETs) based on vapour deposited small molecules. We used diindenoperylene (DIP) as donor (D) and N,N'-bis-(2-ethylhexyl)-1,7-dicyanoperylene-3,4:9,10-bis(dicarboxyimide) (PDIR-CN_2) as acceptor (A) and fabricated D/A as well as A/D heterostructure FETs and used additionally two different contact materials, tetrathiafulvalene tetracyanoquinodimethane (TTF-TCNQ) and aluminum, for preferred hole and electron injection into DIP, respectively. DIP deposited on thermally treated and smoothed tetratetracontane [1] exhibits a electron as well as a hole field-effect mobility μ in the range of $0.1\,\mathrm{cm}^2/\mathrm{Vs}$, whereas PDIR-$CN_2$ shows only e-transport with μ in the same range. As reported previously [2] partial ground state CT between DIP and PDIR-CN_2 molecules takes place resulting in significant changes in the transistor characteristics. In total, we have identified five different working regimes of heterostructure FETs. Temperature dependent measurements of the mobility in the donor and the acceptor indicate among others a significant difference between hole and electron transport in DIP.

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

[2] V. Belova et al. *J. Am. Chem. Soc.* **139** (2017) 8474.

CPP 46.23 Wed 11:00 Poster A

Conjugated polymers with alternating benzothiadiazole-diketopyrrolopyrrole units for OTFTs: Synthesis and DFT/MD simulations — •René Daniel Méndez López[1,2], Deyan Raychev[1,2], Anton Kiriy[1], Olga Guskova[1,2], and Jens-Uwe Sommer[1,2,3] — [1]Leibniz IPF — [2]DCMS, TU Dresden — [3]Institute for Theoretical Physics, TU Dresden

Organic semiconducting polymers are adequate for large area and low cost electronic device applications, such as organic thin film transistors (OTFTs). The joint theoretical/experimental studies are crucial for understanding the charge transport in ambipolar OTFTs, in which both electrons and holes are mobile. Here we report on the synthesis, characterization and simulations of a polymer consisting of diketopyrrolopyrrole (DPP) and benzothiadiazole (B) units. DPP is a versatile building block for OTFTs and its synthesis is straightforward and inexpensive. The π-π intermolecular interactions, the solid-state packing, and optical properties are dependent on the nature of the conjugated blocks adjacent to DPP core. Here, furan (F) is proposed as such an adjacent unit, linking DPP and B blocks in the conjugated backbone. The synthesis of the PDPP-FBF copolymer was performed following Ref.1. From the experiments, the π-π distance, the HOMO-LUMO energy levels and the charge carrier mobilities are characterized. These values are compared with the results of simulations in order to get a deeper understanding of the parameters governing the mobility. This work is funded by ERDF and Free State of Saxony via ESF project CoSiMa 100231947.[1] P. Sonar et al. Chem. Commun., 2012, 48, 8383.

CPP 46.24 Wed 11:00 Poster A

Investigating the influence of morphology on the charge-carrier mobility in organic field-effect transistors — •Tobias Meier[1], Heinz Bässler[1,2], and Anna Köhler[1,2] — [1]Experimental Physics II, University of Bayreuth, 95440 Bayreuth, Germany — [2]Bayreuth Institute of Macromolecular Research, University of Bayreuth, 95440 Bayreuth, Germany

For organic semiconductors it is well known that the charge-carrier mobility depends sensitively on the morphology of the organic semiconductor film. The charge-carrier mobility, however, is one of the most important properties for the application of organic semiconductors as it determines the performance of devices such as organic solar cells and field-effect transistors (OFETs). Yet, there is no comprehensive theoretical description available for this complex morphology-mobility relationship. Here, we use a kinetic Monte Carlo model to simulate charge transport in OFETs in order to investigate the interplay between the morphology of the semiconductor and the charge-carrier mobility. We focus on the role of conjugation length in the charge transport process and on the importance of ordered domains. Parameters considered include the temperature dependence, charge-carrier concentration and film thickness.

CPP 46.25 Wed 11:00 Poster A

Flexible all-carbon solution-gated FETs for pH sensing — •Daniel Hüger[1], David Kaiser[1], Christof Neumann[1], Ugo Sassi[2], Matteo Bruna[2], Maria Küllmer[1], and Andrey Turchanin[1] — [1]Institute for Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Nokia Bell Labs, Cambridge CB3 0FA, UK

Flexible electronics have shown extensive applications in the areas of biology, chemistry, and medicine. We employ single-layer graphene (SLG) grown by methane Chemical Vapor Deposition on Cu foils transferred on PEN substrates and amino-terminated 1 nm thick carbon nanomembranes (CNMs) generated by electron-beam induced crosslinking of aromatic self-assembled monolayers to engineer hybrid NH_2-CNM/SLG field effect transistors. Passivation of the electrodes for the operation of the devices in liquid is realized by self-assembly of hexadecanethiol on the Au contacts. We present the results achieved with these van der Waals heterostructure devices in solution-gated field effect transistors for pH-sensing and compare their performance to that of devices realized on standard SiO_2/Si substrates.

CPP 46.26 Wed 11:00 Poster A

Imidazo[1,5-a]pyridine und -quinoline as a New Class of Materials for Light Emitting Devices — •Jasmin Martha Herr[1,3], Georg Albrecht[2,3], Hisao Yanagi[3], Derck Schlettwein[2], and Richard Göttlich[1] — [1]Institute of Organic Chemistry, JLU Giessen, Germany — [2]Institute of Applied Physics, JLU Giessen, Germany — [3]Nara Institute of Science and Technology, Japan

1,3-disubstituted imidazo[1,5-a]pyridines are receiving increased interest for applications as organic semiconductor thin films, mainly regarding organic light emitting diodes (OLED). Characteristic for these molecules is a blue luminescence with a large Stokes shift and high quantum yields (QY).[1,2] The goal of this work is to explore the potential of this class of materials by introducing specific electron-withdrawing or electron-donating substituents to the chromophore system. A microwave-assisted one-pot synthesis was developed for this purpose which provides a simple and affordable approach towards this new and interesting class of materials. Thin films were prepared by physical vapor deposition (PVD) onto quartz glass. These films and solutions of the molecules were investigated by UV-Vis and fluorescence spectroscopy, as well as lifetime measurements of the excited state to then compare the measurements in solution to those in the solid phase. [1] G. Volpi, G. Magnano, I. Benesperi, D. Saccone, E. Priola, V. Gianotti, M. Milanesio, E. Conterosito, C. Barolo and G. Viscardi, *DyesPigm.* **2017**, 137, 152-164. [2] F. Shibahara, R. Sugiura, E. Yamaguchi, A. Kitagawa and T. Murai, *J.Org.Chem.*, **2009**, 74, 3566-3568.

CPP 46.27 Wed 11:00 Poster A

Optimization and Characterization of Blue OLEDs based on Molecular TADF Emitters — •Felix Klingert[1], Nikolai Bunzmann[1], Sebastian Weissenseel[1], Andreas Sperlich[1], Nikita Drigo[2], Mohammad Khaja Nazeeruddin[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Group for Molecular Engineering of Functional Materials, EPFL, CH-1951 Sion, Switzerland — [3]Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

Realizing efficient and stable blue organic light emitting diodes (OLEDs) that meet display requirements has proven to be a challenging endeavor. Most organic molecules with a bandgap big enough to emit blue light suffer from either poor efficiency or a short lifespan. A modern approach of increasing efficiency is a process called thermally activated delayed fluorescence (TADF). Here, we fabricate blue OLEDs through thermal evaporation based on a molecular TADF emitter and characterize them by means of their current-electroluminescence-voltage characteristics, emission spectra and external quantum efficiency. From these measurements we draw conclusions about the electro-optical properties of the emitter molecules and their suitability as a material for blue OLEDs.

CPP 46.28 Wed 11:00 Poster A

Solution-processed Dual Wavelength Organic Near-Infrared Photodetectors — •Yazhong Wang, Zheng Tang, Bernhard Siegumund, Zaifei Ma, Johannes Benduhn, Donato Spoltore, and Koen Vandewal — Technische Universität Dresden, Nöthnitzer Str. 61, 01187 Dresden, Germany

Optical sensors that are capable of detecting photons at two or multiple specific wavelengths are highly interesting because they can identify target objects or materials much more precisely by detecting the reflected, transmitted or emitted photons at two or multiple characteristic wavelengths. In this work, optical simulations using Transfer Matrix Method (TMM) were performed on organic devices to achieve dual wavelength narrowband detection in the near-infrared spectral range of 700 ~ 1100 nm. The devices exploit charge-transfer (CT) states, formed at the interface of blended organic donating and accepting materials. Combined with a Fabry-Pérot resonant cavity, the CT absorption can be dramatically enhanced at certain wavelengths. Our results show that two detection wavelengths can be tuned independently from 650 to 1100 nm. The spectral resolution (full width at half maximum - FWHM) of the detection bands varies between 10 and 30 nm, and we achieved peak EQEs above 10%. A possible application of such photodetectors is moisture detection, where two of the characteristic absorption peaks of water are located at around 750 and 960 nm. By optimizing the thickness of the two photo-absorbing layers in a tandem device structure, the detection bands can be tuned to match with those two wavelengths for simultaneous and precise detection.

CPP 46.29 Wed 11:00 Poster A

Printed fullerene free organic thin films films for photovoltaic applications — •Rodrigo Delgado, Sebastian Grott, and Peter MüllerBuschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

During the past decade, organic photovoltaics (OPVs) have attracted considerable attention owing to their outstanding characteristics, such as potential low-cost fabrication, high throughput, light weight, flexibility and easy processability. Fabrication techniques for these OPVs devices vary depending on the materials used, and include vaccum evaporation, spin-coating, inkjet printing, doctor-blading, spray casting, screen printing and roll-to-roll printing. Among these, the scalability of the printing processes makes them attractive for industrial application. In this study, the influence of different ratios of donor:acceptor PBDB-T:ITIC for thin film bulk heterojunction (BHJ) OPVs deposited by printing methods are explored. In order to characterize these solar cells their current-voltage characteristics as well as their absorbance spectra are measured. Additionally, the inner morphology of the active layers is probed with advanced scattering techniques, to correlate structure information with the obtained photoelectrical properties of the devices.

CPP 46.30 Wed 11:00 Poster A

A comparative study of thin organic layers for photovoltaic applications using spin and spray coating — •Debamitra Chakraborty, Sebastian Grott, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Bulk-heterojunction organic solar cells have emerged as a promising alternative for conventional silicon based solar cells because of their potential to be light weight, flexible and semi-transparent, which makes them versatile for many applications. Though the most popular scientific method of processing solar cell is spin coating, they can also be processed with solution based methods which enables the possibility to use low cost manufacturing processes like roll-to-roll printing or spray casting. In this study we investigate thin films of different mixtures of conjugated polymers and small acceptor molecules forming organic bulk hetero junctions, which were processed by spin coating or spray casting. Thereby we want to investigate the influence of the different processing techniques on the film morphology and photophysical properties. The structure is analyzed with scattering techniques and correlated with the obtained photophysical properties.

CPP 46.31 Wed 11:00 Poster A

Investigation of low band-gap polymers for highly efficient organic solar cells — •Christoph Bilko, Franziska C. Löhrer, and Peter Müller-Buschbaum — TU München, Physik Department, LS Funktionelle Materialien, 85748 Garching

In contrast to silicon-based solar cells, organic photovoltaics offer a wide range of advantages. Due to their flexibility and tunable optical properties, sun harvesting in areas not accessible to conventional solar cells could be greatly increased using organic solar cells, e.g. on curved or flexible surfaces. Other advantages are the lighter weight and potentially lower production costs. In the last years, the formerly poor efficiencies of organic photovoltaics have been greatly increased. However, further improvements in the device architecture and stability are needed to reach industrially relevant efficiencies. To enhance the performance of solar cells, recent research efforts focus on identifying new highly efficient materials. One way to achieve this is the development of low band-gap polymers, which absorb light of lower energies and can, therefore, increase the overall absorption. Prominent representatives for these kinds of polymers are PTB7 and its derivatives, which can achieve efficiencies of over 10 %. Our work focuses on the comparison of different low band-gap polymers regarding their optical and structural properties. Applied characterization techniques include optical absorption and microscopy measurements as well as X-ray scattering methods. Exploratory solar cells link the power conversion efficiency to parameters such as the active layer composition and morphology.

CPP 46.32 Wed 11:00 Poster A

Investigation of novel material systems for increasing the efficiency of organic solar cells — •Christian Weindl, Franziska C. Löhrer, and Peter Müller-Buschbaum — TU München, Physik Department, LS Funktionelle Materialien, 85748 Garching

In the last decade, interest in organic photovoltaics has increased strongly with enhanced performance values. Even though organic solar cells cannot compete with conventional solar cells in terms of efficiency and long-term stability yet, they have reached the point of industrial application due to a range of unrivaled advantages. Apart from their light weight and their highly tunable optical and mechanical properties, organic solar cells can be produced in an easy and cheap, solution-based way which offers the possibility of mass production via roll-to-roll processing. Their advantages play a particular role in areas not accessible for conventional solar cells, such as curved, flexible or transparent surfaces as well as mobile devices. In our work, we investigate novel material systems used to increase the performance of organic solar cells in terms of efficiency as well as long-term stability. Here, we present insights into the correlation of optical and morphological properties of polymer-based organic photovoltaics by combining real-space imaging and X-ray scattering techniques with optical spectroscopy.

CPP 46.33 Wed 11:00 Poster A

Spontaneous generation of interlayers in OPVs with silver cathodes using additives in a P3HT:PCBM layer — Basel Shamieh[1], Gitti Frey[1], and •Uwe Vogel[2] — [1]Israel Institut of Technology, Haifa 32000, Israel — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

We report a new efficient methodology for processing interlayers by the spontaneous segregation of an additive to a silver cathode. The driving force for this special migration is the chemical interaction between the thiol end group of the additive HEG-DT and the silver. In addition, we report modification of the silver work function at the interface and effectively increase the device Voc which enhances the device efficiency by 76%.

CPP 46.34 Wed 11:00 Poster A

Morphological Investigations on fullerene-free bulk heterojunction blends for photovoltaic applications — •Sebastian Grott[1], Lorenz Biessmann[1], Nitin Saxena[1], Wei Cao[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Elettra-Sincrotrone Trieste, 34149 Basovizza, Italy

Organic solar cells have been in the focus of research for decades due to their advantages in versatility, flexibility, low-cost manufacturing processes, like roll-to-roll-printing, and the tuneable characteristics. These properties open up a wide field of applications and represent an alternative for conventional photovoltaics. Even though the power conversion efficiency is lower than the ones of conventional, values over 11% have been reported. In particular, fullerene-free bulk heterojunction (BHJ) blends receive an increasing attention. We investigate the inner morphology of such BHJ systems. Different compositions of PBDB-T and ITIC BHJ films are studied with advanced x-ray scattering techniques. The obtained structure information is correlated with current density-voltage characteristics and the absorbance of the active layers.

CPP 46.35 Wed 11:00 Poster A

Improvement of Organic Solar Cell Morphology and Device Operation due to Controlled Polymer Aggregation in Solution — •Shahidul Alam[1,2], Rico Meitzner[1,2], Christian Kästner[3], Christoph Ulbricht[4], Daniel A. M. Egbe[4], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany — [2]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldstrasse 10, 07743 Jena, Germany — [3]Institute of Thermodynamics and Fluid Mechanics, Technische Universität Ilmenau, Am Helmholtzring 1, 98693 Ilmenau, Germany — [4]Institute of Polymeric Materials and Testing, Johannes Kepler University, Altenbergerstr. 69, 4040 Linz, Austria

Aggregation of organic semiconductors (OS) generally positively impacts the device performance of polymer solar cells. Aggregation and specifically intermolecular electronic coupling leads to extended absorption spectra by formation of new absorption bands. In addition, more ordered domains of OS improve the free charge carrier generation yield and also reduce recombination rates of free charges located in the ordered phases due to energy relaxation within. Thus, aggregation enhances charge carrier mobility and lifetime, resulting in an improved charge extraction under operating conditions. Here we report progress in controlling polymer aggregation in solution by introduction of antisolvent additives. The impact of polymer aggregation on photovoltaic performance was investigated by various spectroscopic methods.

CPP 46.36 Wed 11:00 Poster A

Investigation of light harvesting complex LHCBM6 for dye-sensitized solar cells — •Fabian Schmid-Michels[1], Nina Lämmermann[2], Olaf Kruse[2], and Andreas Hütten[1] — [1]Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany — [2]Faculty of Biology, Algae Biotechnology & Bioenergy, Bielefeld University, Germany

Light harvesting complexes (LHC) or antenna complexes participate in photosynthesis by harvesting sunlight and transferring the excitation energy to the reaction centre. By channelling this energy elsewhere it is possible to use LHC either as a dye for dye-sensitized solar cells or as energy harvesters for artificial photosynthesis (AP). Solving this challenge could lead to a more efficient regenerative fuel production. To investigate LHCBM6, dye sensitized solar cells were prepared on ITO glass with the LCHs bound to TiO2 nanoparticles. Different binding types were evaluated by electrical measurements and microscopy. Long-term electrical measurements provide insight into the long-term stability.

CPP 46.37 Wed 11:00 Poster A

Composition control and photovoltaic properties of binary polymer:fullerene blends — •Lorena Perdigón-Toro[1], Yueqi Yang[1], Elisa Collado-Fregoso[1], Harald Ade[2], and Dieter Neher[1] — [1]University of Potsdam, Institute of Physics and Astronomy, Germany — [2]Department of Physics and ORaCEL, North Carolina State University, Raleigh, North Carolina 27695, USA

Organic solar cells consist of blends of two or more semiconductors with distinct electronic structures, namely electron donors and acceptors. The morphology of the blend can vary greatly depending on numerous conditions, such as the nature of the materials or the processing. When employing an amorphous polymer and small molecules such as fullerenes, the morphology comprises at least two phases: one phase nearly pure in fullerenes and a second where the macromolecules and fullerenes are intimately intermixed. The initial polymer:fullerene ratio and the annealing temperature play deciding roles on the composition of these two phases. Recent work suggested an unique dependence of the fill factor of solar cells made from binary blends with composition contrast.

In this work, we use PCDTBT:PC71BM as reference to obtain a system ranging from a well-separated blend to a one phase blend. Devices annealed above the critical temperature exhibit much lower fill factor, pointing to increased geminate and/or non-geminate recombination. Various techniques such as bias assisted charge extraction (BACE) and time delayed collection field (TDCF) are used to disentangle these processes and analyse field-assisted charge generation and extraction.

CPP 46.38 Wed 11:00 Poster A

Influence of PMMA protection layers on Ozone degradation of P3HT and MDMO-PPV — •Andreas Frueh[1], Hans-Joachim Egelhaaf[2], Heiko Peisert[1], and Thomas Chassé[1] — [1]Universität Tübingen, IPTC, Auf der Morgenstelle 18 D-72076 Tübingen, Germany — [2]ZAE Bayern, Auf AEG, Bau 16, 1. OG, Fürther Str. 250, D-90429 Nürnberg

The fast degradation of organic polymer materials remains a major problem in organic electronics and optoelectronic devices. We study the influence of PMMA cover layers on the photo oxidation and the degradation by ozone of two prototype polymers: poly(3-hexylthiophene) (P3HT) and Poly[2-methoxy-5-(3*,7*-dimethyloctyloxy)-1,4-phenylenevinylene] (MDMO-PPV) using optical spectroscopies. PMMA films with layer thicknesses of for example 65 nm slow the ozone-degradation down by a factor of 2600. PMMA films do not provide protection against photo oxidation at AM 1.5 in dry or humidified synthetic air.

CPP 46.39 Wed 11:00 Poster A

Printed films of conjugated polymers and small acceptor molecules — •Kerstin Wienhold and Peter Müller-Buschbaum — TU München, Physik Department, LS Funktionelle Materialien, 85748 Garching

Organic photovoltaics are a promising alternative to conventional silicon solar cells as they offer several potential advantages e.g. low weight, high mechanical flexibility and low-cost production. Resent research focuses on identifying new high-efficiency polymers and acceptor molecules to reach high power conversion efficiencies (PCEs). To date, a PCE of 13% could be obtained with a PBDB-T-SF: IT-4F based organic solar cell devices. The fluorinated conjugated polymer PBDB-T-SF acts as a donor whereas the fluorinated small molecule IT-4F acts as an electron acceptor. Both molecules are promising for photovoltaic applications as they show higher absorption coefficients, higher efficiency in exciton separation and charge transport as well as enhanced chemical stability as compared with their non-fluorinated counterparts. However, before commercialization, the solar cell performance must be optimized and an up-scale of the thin layer deposition is necessary. Printing of the individual layers of the solar cells can overcome the up-scale challenge. We print thin PBDB-T-SF: IT-4F films. Characterization techniques such as UV/Vis spectroscopy, photoluminescence and scattering methods such as GISAXS and GIWAXS are applied to get a deeper insight into the composition and morphology of the active layer of the printed films with the aim to further improve the solar cell efficiencies.

CPP 46.40 Wed 11:00 Poster A

Charge transport in layered organic semiconductors — •Anirban Mondal and Denis Andrienko — Max Planck Institute for Polymer Research, Mainz, Germany

Modern organic electronic devices comprise of many semiconducting layers. The performance of these heterostructures is predominantly determined by the relative alignment of ionization potentials and electron affinities in each layer with respect to each other. Despite the continued scientific interest, predicting energy-level alignment at organic heterointerfaces is still a challenge in computational materials science. Using the adapted to charge systems Ewald summation technique and exploring the long-range nature of the charge-multipole interactions, we demonstrate that the density of states is a function of layer thickness and the environment in which this layer is embedded. These results contribute to the understanding of functional heterointerfaces for organic light emitting devices.

CPP 46.41 Wed 11:00 Poster A

Charge Localisation and Quantitative Chemical p-Doping in Single-Wall Carbon Nanotubes — •Bernd Sturdza[1], Michael Auth[1], Klaus H. Eckstein[2], Florian Oberndorfer[2], Andreas Sperlich[1], Tobias Hertel[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Institute of Physical and Theoretical Chemistry, Julius Maximilian University of Würzburg, 97074 Würzburg — [3]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Single-Wall Carbon Nanotubes (SWNTs) meet the requirements for various applications due to their particular electronic properties. As in other semiconductors the influence of defects and doping is highly important for future technologies. Recent studies indicated charge carrier localisation in $AuCl_3$ doped (6,5) SWNTs implied by changing exciton dynamics using indirect all-optical measurements [1]. Here we show direct quantitative studies of p-doping in SWNTs employing electron paramagnetic resonance (EPR). By comparison to a spin count reference sample quantitative EPR yields direct access to doping concentrations. We were able to quantify the p-doping concentrations on the SWNTs for various doping ratios, further receiving new insight into charge carrier confinement.

[1] Eckstein et al., Localized Charges Control Exciton Energetics and Energy Dissipation in Doped Carbon Nanotubes, ACS Nano 2017, DOI:10.1021/acsnano.7b05543

CPP 46.42 Wed 11:00 Poster A

Modeling morphologies with liquid crystalline order in copolymers with conjugated blocks — •Jianrui Zhang, Kurt Kremer, and Kostas Daoulas — Max Planck Institute for Polymer Research, Mainz, Germany

Block copolymers (BCP) with conjugated blocks are interesting for organic electronics. Because of the π-π stacking interactions between aromatic rings in the backbone and short side chains, conjugated blocks can form liquid crystals (LC) with collective planar order or crystalline phases. Therefore, the phase behavior of BCP with conjugated blocks is significantly more complex comparing to classical BCP and their properties are less understood. Here we investigate the effects of collective planar order on conformational and structural properties of these materials. For this purpose, we employ a generic model, where conjugated blocks can create collective planar order characterized by biaxial nematic symmetry. We consider diblock copolymers consisting of one flexible and one conjugated block, and restrict our study to the simplest case – lamellar phase. First Monte Carlo (MC) simulations in the canonical ensemble are used to locate approximately the region of the parameter space where lamellae are formed. Then variable box-shape MC simulations are performed to find optimized lamellae with uniform stress. The optimized lamellae comprise alternating amorphous and biaxial layers, formed by flexible and conjugated blocks respectively. Interestingly, we find that different biaxial layers have the same preferred chain alignment direction but different π-stacking directions. This observation indicates decorrelation between biaxial layers.

CPP 46.43 Wed 11:00 Poster A

Influence of Morphology on Mobility in Perylene Bisimide Polymer Systems — •Hazem Bakr[1], Julian Kahle[1], Mukundan Thelakkat[2], and Anna Köhler[1,3] — [1]Experimental Physics II, Uni Bayreuth — [2]Macromolecular Chemistry I, Uni Bayreuth — [3]BIMF, Uni Bayreuth

We investigate how morphological and conformational order affects the charge transport in two different perylene bisimide (PBI) based polymers. The two PBIs used differ in their sidechains, thus leading to different morphologies. Time resolved photoluminescence measurements in solution and film have shown the presence of two emitting species, present at different amounts. A long lived one with a lifetime of 20 ns which is attributed to excimer emission and a short lived one with a lifetime of 4 ns assigned to the PBI monomer emission. Using electron only devices, we determine the electron mobility using space charge limited current (SCLC) measurements. The differences in charge mobilities and their relation to the film morphology are discussed.

CPP 46.44 Wed 11:00 Poster A

Efficient doping of poly(3-hexylthiophene) using the strong Lewis acid tris(pentafluorophenyl)borane — •Malavika Arvind[1], Patrick Pingel[2], Christian Röthel[3], Silvia Janietz[2], Ingo Salzmann[4], and Dieter Neher[1] — [1]University of Potsdam, Germany — [2]Fraunhofer Institute for Applied Polymers, Germany — [3]Karl-Franzens Universität Graz, Austria — [4]Humboldt Universitaet zu Berlin, Germany

Molecular doping provides a convenient way of improving the conductivity and transport properties of organic materials. In this study, we use tris(pentafluorophenyl)borane (BCF)- a well soluble, strong Lewis acid that is known to serve as a p-dopant[1], to dope the semiconducting polymer poly(3-hexylthiophene) (P3HT). Analysis of the sub-band gap signals in the UV-Vis-NIR spectra of BCF doped P3HT solutions and thin films indicates a doping process similar to that in F4TCNQ-P3HT, despite the obvious structural dissimilarity between the two dopants.[2] However, grazing incidence x-ray diffraction (GIXRD) experiments reveal important differences between the two systems. While co-crystal formation is observed in F4TCNQ-P3HT films[3], such features are absent in the BCF-P3HT system. By employing different techniques for film preparation and doping, we succeeded in fabricating doped films with high structural homogeneity and outstanding electrical conductivities.

[1] Welch et al., J. Am. Chem. Soc., 133 (2011) 4632

[2] Pingel, Arvind et al., Adv. Electron. Mater., (2016) 2: 1600204

[3] Mendez, Salzmann et al. Nat. Comm., (2015), 6, 8560

CPP 46.45 Wed 11:00 Poster A

Drift, Diffusion, and Immobilization of Organic Dopant Molecules - Challenges and Prospects — •Sebastian Beck[1,2], Patrick Reiser[2,3], Heiko Mager[1,2], Vipilan Sivanesan[1,2], Jakob Bernhardt[1,2], Frank Simon Benneckendorf[2,4], Lars Müller[1,2,5], and Annemarie Pucci[1,2] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]InnovationLab, Heidelberg — [3]Surface Science Devision, TU Darmstadt — [4]Organisch-Chemisches Institut, Universität Heidelberg — [5]Institut für Hochfrequenztechnik, TU Braunschweig

A precise adjustment of dopant distribution is crucial for the functionality of organic electronic devices. Therefore, a lot of effort is made to control the molecular composition in devices throughout fabrication. However, diffusion processes as well as drift of organic dopant molecules can alter the carefully planned device architecture resulting in device fatigue. Therefore, detailed studies of diffusion and drift properties as well as a method to immobilize organic dopant molecules are needed to further improve device performance. In this study, the drift of dopant molecules, such as F4TCNQ and Mo(tfdCO2Me)3, in external electric fields was investigated. IR micro-spectroscopy of doped P3HT layers in combination with electrical measurements was used to clarify the underlying processes. Additionally, the diffusion properties of Mo(tfdCO2Me)3 in sequentially doped P3HT layers with varying regioregularity were studied by in-situ IR and Photoelectron spectroscopy. We further present an UV triggered immobilizing procedure and introduce it to derivatives of the n-type dopant N-DMBI.

CPP 46.46 Wed 11:00 Poster A

Exploring the design of a complex and versatile Kinetic Monte Carlo code, for organic electronics applications — •Leanne Paterson and Denis Andrienko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

There is a vast and continuously growing interest in the field of organic electronics. Although in it's infancy with respect to inorganic competitors, it is clear that the use of organic materials in electronic devices can offer a cheaper, flexible and highly variable alternative. In order for the field to advance and maximise the capabilities of such devices, it is vital to understand the molecular processes involved. Kinetic Monte Carlo (KMC) simulations offer a method to investigate the movement of charge carriers through the organic material, with the possibility to incorporate effects such as recombination of carriers and coulomb interaction. Charge carrier movement in organic semiconductors can be described via a "hopping" mechanism. Each carrier hop or event, takes the system from state "a" to "b", there is a corresponding rate for this transition and a probability for it to occur, which can be represented by the master equation. KMC is one method of solving this master equation, giving a randomly generated trajectory of carrier movement within the organic material. The KMC code presented, uses a two-level variable step size method (VSSM) algorithm, to increase computational efficiency. The algorithm proceeds with pre-computed rates, calculated using Marcus theory, which are grouped corresponding to carrier type and position.

CPP 46.47 Wed 11:00 Poster A

Structural models of the n-type nickel-tetrathiooxalate polymers: A combined DFT/MD approach — Roman Tkachov[1,2], Lukas Stepien[2], Robert Grafe[2], •Olga Guskova[3], Anton Kiriy[3], Heiko Reith[4], and Christoph Leyens[1,2] — [1]TUD, Helmholtzstr. 7, 01062, Dresden — [2]Fraunhofer IWS, Winterbergstr. 28, 01277, Dresden — [3]IPF Dresden, Hohe Str. 6, 01069, Dresden — [4]IFW Dresden, Helmholtzstr. 20, 01069, Dresden

In this work, the 3D models of the n-type nickel-tetrathiooxalate polymers poly(Ni-tto) and poly[Kx(Ni-ett)] have been studied for the first time using DFT, the crystal packing prediction, all-atom MD simulations and experiments [1,2]. As a result, possible unit cells for both polymers are suggested, having densities and the XRD patterns close to the experimental ones [2]. The predicted 3D packings consist of two structural elements: the π-stacked columns and the herringbone arrangements with counterions intercalating in-between stacks. From the all-atom MD simulations, the close contacts S...Ni, S...S, the distributions of counterions and the thermal disorder are characterized. This distinguishes our approach from the previously reported ones either on a linear idealistic chain [3] or on 3D models without counterions [4]. We are currently focusing on the calculations of the Seebeck coefficient for 3D models of polymers as promising elements for thermoelectric applications. This work is supported by SAB (Proj.100245366) and AiF (IGF-Proj.18165BR). [1] R. Tkachov et al Tetrahedron, 2017, 73, 2250. [2] R. Tkachov et al Polym. Chem., 2017 (submitted). [3] D. Tiana et al PCCP, 2014, 16, 14463. [4] T. Vogt et al JACS 1988, 110, 1833.

CPP 46.48 Wed 11:00 Poster A

LT-UHV-STM investigations on single benzylnaphthoic diimides adsorbed on metal(111)-surfaces — •Bertram Schulze Lammers[1], René Ebeling[1], Elena Dirksen[2], Thomas J. J. Müller[2], and Silvia Karthäuser[1] — [1]Peter Grünberg Institut (PGI-7) and JARA-FIT, Forschungszentrum Jülich GmbH, Germany — [2]Institut für Organische Chemie und Makromolekulare Chemie, Heinrich-Heine-Universität Düsseldorf, Germany

LT-UHV-STM investigations allow the detailed characterization of the adsorption behavior and the geometry of 2-dimensional molecules physisorbed on atomically flat surfaces up to their orbital structure. As functionalized naphthalene diimides (NDIs) received current interest due to their possible use as small molecular acceptors for various applications in molecular electronics, we deduced the adsorption behavior and the electronic behavior of these molecular compounds by STM. Here the 2,7-dibenzyl 1,4,5,8-naphthalenetetracarboxylic diimide (BNTCDI), which consist of a large π-conjugated NDI backbone and two benzyl-groups connected to the central part, have been studied as prototypical 3-dimensional NDI compounds. Recent results [1] for BNTCDI on the Pt(111)-surface verified the 3-dimensional structure of the adsorbed molecule with the phenyl groups standing vertically with their phenyl plane on the substrate. In addition to these results the electronic and topographic structure of BNTCDI adsorbed on different (111)-surfaces was investigated in detail and compared to DFT based calculations on BNTCDI in the gas phase and its orbital symmetry of the HOMO and the LUMO. [1] DOI: 10.1021/acs.jpcc.7b09911

CPP 46.49 Wed 11:00 Poster A

Spin crossover iron(II) coordination polymer with fluorescent properties: correlation between emission properties and spin state — Charles Lochenie[1], •Konstantin Schötz[2], Fabian Panzer[2], Hannah Kurz[1], Bernadette Maier[1], Florian Puchtler[4], Seema Agarwal[5], Anna Köhler[2,3], and Birgit Weber[1] — [1]Inorganic Chemistry II, Universität Bayreuth — [2]Experimental Physics II, Universität Bayreuth — [3]Bayreuth Institute of Macromolecular Research, Universität Bayreuth — [4]Inorganic Chemistry I, Universität Bayreuth — [5]Macromolecular Chemistry II, Universität Bayreuth

Spin crossover complexes show great potential as molecular switches or data storage devices. For a good performance as such, the switching between the high spin (HS) and the low spin (LS) state should be abrupt and show a stable hysteresis in an accessible temperature region. We report the synthesis and characterization of a spin crossover coordination polymer exhibiting such attributes. By differential scanning calorimetry and magnetic measurements, Mössbauer spectroscopy, and X-ray powder diffraction, we revealed a wide and stable hysteresis of the spin transition between $T_{1/2,\ up} = 371\ K$ and $T_{1/2,\ down} = 323\ K$, which can additionally be tracked using photoluminescence spectroscopy due to a change in emission color.

CPP 46.50 Wed 11:00 Poster A

Phosphorescence Lifetime of a Brominated Diphenylphosphine-Alkyl Naphthaleneimide Luminescence Turn-On Dyad in Different Atmospheres — Sebastian Feulner[1], •Lothar Kador[1], Paul M. Reichstein[2], and Werner Reichstein[3] — [1]University of Bayreuth, Institute of Physics, 95440 Bayreuth, Germany — [2]University of Bayreuth, Macromolecular Chemistry I, 95440 Bayreuth, Germany — [3]University of Bayreuth, Bayreuth Materials Center (BAYMAT), 95440 Bayreuth, Germany

We have studied a brominated diphenylphosphine-alkyl naphthaleneimide luminescence turn-on dyad which, in its oxidized form, emits strong fluorescence and moderate phosphorescence when excited with UV light at 365 nm. In ambient air, the phosphorescence is partly quenched by triplet-triplet annihilation (TTA) with molecular oxygen. At lower pressure, TTA is reduced and, therefore, the contribution of the phosphorescence to the total luminescence and the phosphorescence lifetime increase. The phosphorescence signal and the phosphorescence lifetime were studied in the frequency domain with modulated UV excitation at air pressures between 1 bar and vacuum. Both quantities increase strongly below 100 mbar. The phosphorescence was also investigated in pure oxygen and pure argon atmosphere at 1 bar. As expected, oxygen causes slightly stronger phosphorescence quenching than air. Surprisingly, in argon the phosphorescence is significantly weaker than in vacuum. The experimental data are interpreted in the so-called polar-plot (or Cole-Cole plot) representation.

CPP 46.51 Wed 11:00 Poster A

Calculation of electron-phonon coupling constants in π-conjugated molecules from first principles — •Irina Petreska[1,2] and Gertrud Zwicknagl[2] — [1]Faculty of Natural Sciences and Mathematics, Ss. Cyril and Methodius University in Skopje, 1000 Skopje, Republic of Macedonia — [2]Institut für Mathematische Physik, Technische Universität Braunschweig, 38106 Braunschweig, Germany

Electron-phonon coupling constants for a class of π-conjugated molecules will be calculated using excited states and vibrational spectra obtained from first principles. Electronic excitations will be evaluated in the frame of configuration interaction (CI) picture, as well as the time-dependent density functional theory (TD-DFT). Hamiltonian matrix involving electronic and vibronic energies obtained from CI and TD-DFT calculations will be then composed, which will enable evaluation of the electron-phonon coupling constants. The obtained results could be further used to parametrize the extended Hubbard-like Hamiltonians in order to treat the inelastic transport regime in π-conjugated molecules.

CPP 46.52 Wed 11:00 Poster A

Singlet And Triplet Dynamics of Covalently Bound Ditetracene in Various Environments — •Maximilian Frank[1], Ulrich Müller[1], Lena Roos[2], Anke Krueger[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Institute of Organic Chemistry, Julius Maximilian University of Würzburg, 97074 Würzburg — [3]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Singlet fission significantly affects the performance of many organic photovoltaic cells and light-emitting diodes. In this process a singlet state decays into two triplet states which strongly depends on the relative orientation of the participating chromophores. As tetracene constitutes a model system showing efficient, thermally activated singlet fission, we study covalently bound ditetracene to determine the influence of the rotation angle between the two tetracene molecules on this process. Therefore, ditetracene and tetracene doped into different host systems like a disordered PMMA matrix or a single anthracene crystal are optically analysed by means of photon-correlation studies together with lifetime measurements at room temperature. By comparing this data with that of a tetracene single crystal or the molecules in solution we are able to identify two different excitonic species in ditetracene and to show how the influence of the environment and temperature affects their photophysical characteristics such as the spectral intensity distribution, fluorescence lifetime and quantum efficiency. This project was funded by the DFG in the framework of the GRK 2112.

CPP 46.53 Wed 11:00 Poster A

Synthesis of a series of brominated TPB molecules to increase the phosphorescence — •Anna Haft[1], Felix Fries[1], Ramunas Lygaitis[2], Olaf Zeika[1], and Sebastian Reineke[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials, TU Dresden, Nöthnitzer Str. 61, 01187 Dresden — [2]Kaunas University of Technology, K. Donelaičio g. 73, 44249 Kaunas

Biluminescent emitter molecules are able to show phosphorescence and fluorescence efficiency at room temperature. N,N,N',N'-tetraphenyl-[1,1'-biphenyl]-4,4'-diamine (TPB) is one of these special emitters. By adding heavy atoms like bromine it is possible to increase the ratio of phosphorescence to fluorescence by increasing the intersystem crossing through intramolecular heavy atoms.

To investigate this effect, a series of TPB derivates was synthesized successfully. The pure TPB was obtained using the Ullmann reaction. A bromination in para position in case of mono to tetra brominated species was achieved via an electrophilic substitution with N-bromosuccinimide. The materials were investigated in form of a host:guest system embedded in a rigid matrix of poly(methyl methacrylate) PMMA with respect to the internal conversion rates, where the increased phosphorescence-to-fluorescence ratio with increasing heavy atom decoration was confirmed.

CPP 46.54 Wed 11:00 Poster A

Macroscopic anisotropic optical properties by wrinkling instabilities — •Anik Kumar Ghosh[1], Bernhard Alexander Glatz[1], Sven Wiessner[1,2], Amit Das[1], Tobias A. F. König[1,2], and Andreas Fery[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e. V., Germany — [2]Cluster of Excellence Centre for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, Germany

Polymeric wrinkled structures are exquisite, concerning their apparent advantages with reverence to their flat counterparts. Their repeating sinusoidal geometry is the result of an energetic instability induced by a mechanical mismatch between two layers that is easy to handle, reproducible and very robust. A well-known way to gain such structures represents the oxidation of a pre-strained polydimethylsiloxane (PDMS) slab by plasma treatment [Microchimica Acta, 2009, 165, 249 and Soft Matter, 2015, 11, 3332]. It creates in situ a glassy layer on top, while the consequent strain relaxation of the two-layer system results in a mechanical buckling instability that forms permanent wrinkles. In our setup, we move onward by fabricating blazed grating structures via angle-dependent thin metal film deposition on top of the PDMS wrinkles. This enables them for enhanced light-matter interactions, subsequently a gateway towards high-performance optoelectronic devices, non-linear optical phenomena which further results in a key point to build a cost-efficient class of photonic structures. Supported by finite-difference time-domain simulations, we further discuss the grating efficiency of the anisotropic structure.

CPP 46.55 Wed 11:00 Poster A

Optical and structural properties of diindenoperylene and perylene-tetracarboxylic-diimide on ZnO and SiO_2 — •Clemens Zeiser, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Germany

In recent years, heterostructures of donor and acceptor compounds have attracted significant attention due to their applications in organic devices [1]. We studied blends of diindenoperylene and perylene-tetracarboxylic-diimide (PTCDI) deposited by organic molecular beam deposition on SiO_2 as an inert and on ZnO as a strongly interactive substrate. Uniaxial absorption spectra of films on silicon oxide measured by spectroscopic ellipsometry could be explained with the molecular structure determined by synchrotron x-ray diffraction. Using differential reflectance spectroscopy, also thickness dependent absorption spectra of films deposited on ZnO and SiO_2 have been examined. We find changes in the vibronic progression of flat-lying monolayer spectra which could be assigned to molecular interactions with the ZnO surface [2]. Furthermore, also the changing absorption spectra of the following layers could be explained by molecular coupling and morphologic influences.

[1] A. Hinderhofer, ChemPhysChem 2012, 13, 628-643

[2] P. Winget et. al., Adv. Mater. 2014, 26, 4711-4716

CPP 46.56 Wed 11:00 Poster A

Investigation of opto-electronic properties of ZnPc:F_4ZnPc OLEDs — •Simon Wiegand[1], Thomas Ferschke[1], Gabriel Freiherr von Eyb[1], Sebastian Hammer[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius-Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

To analyze the electrically driven generation of excitonic and possible charge transfer states we fabricated organic light emitting diodes (OLEDs) comprising an emission layer (EML) made out of co-evaporated neat and partially fluorinated zinc phthalocyanin, ZnPc and F_4ZnPc, respectively. By means of electroluminescence (EL), photoluminescence (PL) and I(V) characteristics, we studied the opto-electronic properties of these OLEDs. The additional variation of the EML thickness provides access to the microscopic mechanisms, such as local space charging or an unbalanced injection of electrons and holes, governing the radiative as well as non-radiative relaxation of excited states. Furthermore, guided by a recent publication of our group [1] we intend to utilize plasmonic emission enhancement by using suited electrode materials and electrode geometries matching the spectral characteristics of our ZnPc:F_4ZnPc OLEDs.

[1] V. Kolb, *et al.*, *Opt Express*, **2017**, 25(6), 6678–6689

CPP 46.57 Wed 11:00 Poster A

Study on conductive silver nanowire networks in 3D printed polymers — •Lewis Akinsinde[1], Tomke Glier[1], Ferdinand Otto[1], Calvin J. Brett[2,3], Milena Lippmann[3], Stephan V. Roth[3,4], and Michael A. Rübhausen[1] — [1]Institut für Nanostruktur und Festkörperphysik, Universität Hamburg — [2]Department of Fluid Physics, Royal Institute of Technology (KTH), Stockholm, Sweden — [3]Photon Science, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [4]Royal Institute of Technology (KTH), Stockholm, Sweden

Nowadays, increasing attention has been devoted to transparent conductive films because of their various applications in Solar cells and OLEDs. 3D printing is an alternative promising fabrication process. The embedding of silver nanowires in a UV sensitive polymer matrix enables 3D printable conductive objects. Hence silver nanowires were synthesized via the polyol method resulting in an average diameter of approximately 130 nm and a length up to 100 μm. With optimization through dry etching sheet electrical resistance could be reduced to ca. 1.5 Ω/square. This is highly competitive with existing candidates such as indium tin oxide (ITO). As a next step layer systems consisting of UV cured 1,6-Hexanediol diacrylate (HDDA) and silver nanowires were prepared. The structure and morphology of the silver nanowire incorporated thin films were investigated by scanning electron microscopy (SEM), atomic force microscopy (AFM), conductivity measurements and spectroscopic measurements. Inner film morphology was studied using grazing incidence small-angle X-ray scattering (GISAXS)

CPP 46.58 Wed 11:00 Poster A

Flexible Modulation of Electronic Band Structures of Wide Band Gap GaN Semiconductors Using Bioinspired, Non-Biological Helical Peptides — •Sven Mehlhose[1], Natalya Frenkel[1], Wasim Abuillan[1], Sara Lippert[3], Gesche Müntze[3], Martin Eickhoff[3], Shunsaku Kimura[2], and Motomu Tanaka[1] — [1]Physical Chemistry of Biosystems, Institute of Physical Chemistry, Heidelberg University, D69120 Heidelberg, Germany — [2]Department of Material Chemistry, Graduate School of Engineering, Kyoto University, 6158510 Kyoto, Japan — [3]Institut für Festkörperphysik, Universität Bremen, Otto-Hahn-Allee, D28359 Bremen

We show the modulation of the electronic band profiles of wide band gap GaN semiconductors by the macromolecular dipole potentials exerted from ordered monolayers of synthetic, non-biological aldehyde terminated helical peptides deposited on wet chemically oxidized GaN surfaces functionalized with aminosilanes. The selective coupling of either N- or C-terminal to the amino-terminated surface enables one to control the direction of the dipole moment. After confirming the formation of highly ordered peptide monolayers, the impact of macromolecular dipole potentials was quantified by electrochemical impedance spectroscopy. The same functionalization steps were transferred to GaN/AlGaN/GaN high electron mobility transistor structures. Stable and quantitative modulation of the current-voltage characteristics of the two-dimensional electron gas by the deposition of bio-inspired peptides is a promising strategy for the macromolecular dipole engineering of GaN semiconductors.

CPP 47: Electrical, Dielectrical and Optical Properties of Thin Films II

Time: Wednesday 12:00–13:00 Location: C 230

CPP 47.1 Wed 12:00 C 230

Aligned in-plane polarization and large piezoelectricity in P(VDF-TrFE) films on graphite — •Robert Roth[1], Martin Koch[1], Jakob Schaab[2], Martin Lilienblum[2], Thomas Thurn-Albrecht[1], and Kathrin Dörr[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, 06099 Halle, Germany — [2]Department of Materials, ETH Zürich, 8093 Zürich, Switzerland

Ferroelectric polymers are attractive candidates for functional layers in electronic devices like non-volatile memories, piezo- and magnetoelectric sensors. However, thin films often reveal reduced di- and piezoelectric responses due to crystalline disorder and resulting non-aligned electrical dipoles leading to compensation effects. One of the best characterized and often applied ferroelectric polymers is poly(vinylidene fluoride-co-trifluoroethylene) (P(VDF-TrFE)). We will present results on aligning both in-plane and out-of-plane ferroelectric polarization in P(VDF-TrFE) films on graphite in a force microscope. Within written micron-sized domains, strong enhancement of both, lateral and vertical piezoresponses have been achieved. Polarization alignment in as-prepared films of several 10 nm thickness is controlled using a combined procedure of electrical poling and mechanical tip pressure. Micron-sized domains with uniform polarization orientation, within the resolution limit, allow one to overcome compensation effects which would be beneficial for various device applications.

CPP 47.2 Wed 12:15 C 230

Optoelectronic properties of Ag clusters on polymer thin films during sputter deposition — •Marc Gensch[1,2], Matthias Schwartzkopf[1], Bjoern Beyersdorff[1], Wiebke Ohm[1], Calvin Brett[1,3], Deniza Checkrygina[2], Pallavi Pandit[1], Andreas Stierle[2], and Stephan Roth[1,3] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]University of Hamburg, Luruper Chaussee 149, D-22761 Hamburg — [3]KTH, Teknikringen 56-58, SE-100 44 Stockholm

Nanostructured polymer-metal-composites demonstrate great perspectives for optoelectronic applications [1], e.g. as sensors or photovoltaics. To enhance properties of such devices the self-assembly process needs to be understood. We studied the insulator-metal transition during sputter deposition of silver on co- and homopolymers by grazing incidence small-angle X-ray scattering (GISAXS) in combination with surface differential reflectance spectroscopy (SDRS) [2]. As templates, solvent annealed highly ordered PS-b-PMMA diblock copolymers and their corresponding homopolymers were used. Our study reveals the selective wetting of silver on one of the polymer blocks and the influence of the template on the percolation behavior of the silver layer. In situ GISAXS measurements indicate a difference in the embedding of silver clusters depending on the polymer template. [1] S. V. Roth et al., ACS Appl. Mater. Interfaces 7, 12470 (2015). [2] M. Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015).

CPP 47.3 Wed 12:30 C 230

Ultra-sensitive guided-mode resonance refractive index sensor — •Swagato Sarkar[1], Tobias A. F. König[2,3], Andreas Fery[2,3,4], and Joby Joseph[1] — [1]Dept. of Physics, Indian Institute of Technology Delhi, New Delhi, India-110016 — [2]Leibniz-Institut für Polymerforschung Dresden e.V., Institute of Physical Chemistry and Polymer Physics, Hohe Str. 6, 01069 Dresden, Germany — [3]Cluster of Excellence Centre for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany — [4]Department of Physical Chemistry of Polymeric Materials, Technische Universität Dresden, Hohe Str. 6, 01069 Dresden, Germany

In this work, an extremely sensitive refractive index (RI) sensor employing phase detection in a guided mode resonance (GMR) structure is presented where the GMR structure is introduced to one of the arms of a Mach-Zehnder Interferometer to detect RI change through phase measurement via fringe shift. The sensitivity comes out to be 0.608π phase shift per 10^{-4} RI change in water medium which is more than 100 times higher than the other reported GMR based phase detection method. Using the experimental set up, a minimum phase shift of (1.94 x 10^{-3}) π can be measured that corresponds to a RI change of 3.43 x 10^{-7}, outperforming the sensitivity of any of the reported optical sensors. Finally, an alternative lithography free approach is considered using directed self-assembly method. Due to the high optical quality of the novel metal building blocks and the up-scalability of the self-assembly method, an outlook towards fabrication of cost efficient GMR ultra-sensitive refractive index sensor will be discussed.

CPP 47.4 Wed 12:45 C 230

Optoelectronic properties of functionalized diamondoids: sensing DNA-nucleotides — •Chandra Shekar Sarap[1], Partovi-Azar Pouya[2], and Maria Fyta[1] — [1]Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Institute of Chemistry, Martin Luther University, Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale), Germany

Diamondoids, the small nanometer-sized hydrogen-terminated hydrocarbon cages or diamond-like structures with sp3 carbon, are complementary to sp2 carbon nanomaterials such as graphene, carbon nanotubes, and fullerenes. Due to their unique molecular framework, these molecules have recently gained a lot of interest that possess high thermal stability, superior chemical resistance, and negative electron affinity making them good candidates for electron emitting devices. Herein, we investigate the performance of functionalized diamondoids as a probe to sense DNA using density functional theory (DFT). We focus on the optical properties of functionalized diamondoids interacting with different nucleotides by considering the hydrogen-bond strength. Moreover, the corresponding charge-transfer time scales between the diamondoids and the nucleotides reveals that the interaction of the diamondoids with different nucleotides results in different optical and charge-transfer properties which in turn can be exploited for detection of the nucleotides. The studies are motivated by the high potential of diamond-based materials for optoelectronic applications as well as sensors for DNA detection.

CPP 48: Focus: Fundamental Physics of Perovskites I - organized by Lukas Schmidt-Mende and Vladimir Dyakonov

Time: Wednesday 15:00–17:45 Location: C 130

Topical Talk CPP 48.1 Wed 15:00 C 130

Long lifetimes and small phonon energies in metal-halide perovskite solar cells — •Thomas Kirchartz[1,2], David Egger[3], and Uwe Rau[1] — [1]IEK5 Photovoltaik, Forschungszentrum Jülich GmbH, 52428 Jülich — [2]Faculty of Engineering and CENIDE, University of Duisburg-Essen, Carl-Benz-Str. 199, 47057 Duisburg, Germany — [3]Institute of Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Lead-halide perovskite solar cells have remarkably high open-circuit voltages and relatively long lifetimes as determined from e.g. transient photoluminescence or transient microwave photoconductivity. These long lifetimes lead to fairly good charge carrier collection properties and in addition a high internal luminescence yield that makes these materials suitable for photovoltaics and other optoelectronic applications. One agreed-upon reason for these long lifetimes is the defect tolerance of lead-halide perovskites and the subsequently low density of deep defects in the material. However, various other potential explanations for long lifetimes and high open-circuit voltages have been brought forward. Among them are the existence of an indirect band gap, low effective masses or polaronic effects. Here, we recall the classical theories for non-radiative recombination via emission of multiple phonons, which predict the capture cross sections as a function of microscopic parameters such as the phonon energy, the deformation potential constant and the frequency dependent permittivity. Based on these theories we discuss the impact of low phonon energies and the strongly frequency dependent permittivity on recombination.

CPP 48.2 Wed 15:30 C 130

Observation of coherent phonons upon photo-excitation in lead halide perovskite — •Vandana Tiwari[1], Hong-Guang Duan[1,2,3], Ajay Jha[1], Pabitra Nayak[4], Michael Thorwart[2,3], Henry Snaith[4], and R. J. Dwayne Miller[1,3,5] — [1]MPSD, Hamburg, Germany — [2]I. Institut für Theoretische Physik, UH, Germany — [3]CUI, Hamburg, Germany — [4]University of Oxford, UK — [5]University of Toronto, Canada

The unprecedented success of hybrid organolead halide perovskites in different cell designs demands the fundamental understanding of underlying microscopic mechanisms for photoinduced charge generation. Electronic dynamics of perovskite upon photo-excitation has provided deep insights into its optoelectronic behavior, but the contribution of lattice vibrations is still to be deciphered. We have employed ultrafast transient grating spectroscopy to probe impulsively excited vibrational modes of CH3NH3PbI3 in thin films. We distinctly observe the ground and excited state vibrational modes at room temperature. The interplay of strongly coupled dominant vibrational modes to ultrafast carrier generation process will be discussed.

CPP 48.3 Wed 15:45 C 130

Impact of Temperature Induced Structural Dynamics on the Optical Properties of Hybrid Perovskites — •Fabian Panzer and Anna Köhler — Experimental Physics II, University of Bayreuth

There is still a need in the field of hybrid perovskites to fundamentally understand how changes in the structure, be it the crystal structure, material composition or surface morphology impact on their electronic structure, i.e. their optical properties. Due to their soft nature, hybrid perovskites are prone to changes in their structure, which, for example, can be induced by changing the temperature of the sample, be it realized by cooling in a cryostat,[1] or by local heating due to laser irradiation.[2] Here we present detailed temperature dependent absorption and photoluminescence characterizations on both, polycrystalline thin films and single crystals of the prototypical perovskite methylammonium lead iodide. From our measurements we distinguish between different crystal structures, phase transitions and investigate the influence of disorder on the electronic structure.[3] Furthermore we identify the existence of additional recombination pathways already in the high temperature tetragonal phase of the material. We show that it is possible to induce this phase also at lowest temperatures by local laser heating. This allows to distinguish between the emission features from distinct crystal phases and defect states, to gain full information about the optical properties of the investigated perovskites.

[1] F.Panzer et al., Adv. Energy Mater, 7, 2017, 1700286; [2] F.Panzer et al., Adv. Optical Mater. 6, 2016, 917; [3] S.Singh, C.Li, F.Panzer et al., J. Phys. Chem. Lett, 7, 2016, 3014

CPP 48.4 Wed 16:00 C 130

The influence of solvent engineering on the fundamental functionality of organolead triiodide perovskite solar cells — •Julian Höcker[2], Philipp Rieder[1], David Kiermasch[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

The organic and hydrophobic polymer poly[N, N'-bis(4-butilphenyl)-N, N'-bis(phenyl)-benzidine] (pTPD) is a representative hole transport layer (HTL) for its use in hybrid perovskite solar cells. Due to its beneficial energy levels, whereby its highest occupied molecular orbital (HOMO) level matches with the valence band level of methylammonium lead iodide perovskite, an efficient hole extraction can be achieved. In this study, we demonstrate highly efficient planar p-i-n perovskite solar cells using pTPD as HTL and CH3NH3PbI3 processed from 2-step interdiffusion as the active layer. We found that the wettability of DMF strongly depends on the preparation method of pTPD. With varying the solvent and material concentrations we increased the wettability of the perovskite layer which lead to an increase in power conversion efficiency (PCE) of the corresponding solar cell devices. Our solvent engineering approach demonstrates that in this case no further interface modifications is needed for the preparation of efficient perovskite solar cell devices.

CPP 48.5 Wed 16:15 C 130

Time-resolved structural analysis of humidity assisted crystallization in printed mesoscopic organometal halide perovskite solar cells — •Oliver Filonik[1], Margret Eva Thordardottir[1,2], Jenny Lebert[2], Stephan Pröller[2], Sebastian Weiss[2], Jia Haur Lew[3], Anish Priyadarshi[3], Nripan Mathews[3], Peter Müller-Buschbaum[2], and Eva M. Herzig[4] — [1]TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [3]Energy Research Institute @ NTU (ERI@N), Research Techno Plaza, 637553 Singapore, Singapore — [4]Universität Bayreuth, Physikalisches Institut, Herzig Group - Dynamik und Strukturbildung, 95440 Bayreuth, Germany

Organometal halide perovskite based solar cells have emerged as the fastest-advancing photovoltaic technology to date. However, in-depth knowledge about the perovskite crystal formation and optimal processing protocols is still lacking. In the presented work, we fabricate a mesoscopic scaffold comprised of a triple-layer of titania, zirconia and carbon by screenprinting. We further investigate the influence of humidity on the perovskite formation inside the scaffold by time-resolved grazing incidence wide angle X-ray scattering. The experimental data reveal the formation of intermediate solvent phases in solution due to humidity, altering the perovskite formation route. Our results grant us a better understanding of the humidity assisted perovskite crystallization processes and are of key importance for further developments.

15 min. break

CPP 48.6 Wed 16:45 C 130

Investigation of Photon Recycling in Perovskites by Spatially-Resolved Confocal Photoluminescence — •Milena Merkel[2], Liudmila Kudriashova[1], Valentin Baianov[2], Simon Berger[1], Georgy V. Astakhov[1], Andreas Baumann[2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Methylammonium lead iodide (MAPI) perovskites were shown to combine long diffusion lengths (up to 10 μm) with high carrier recombination rates ($\sim 10^6\ s^{-1}$). Coexistence of these competing properties can be explained by efficient interplay between photons and electron-hole pairs in the perovskite film with multiple absorption-diffusion-emission events occurring, namely by photon recycling. Here we implement confocal double-objective photoluminescence (PL) spectroscopy to study the photon recycling in MAPI. Analysis of steady-state PL spectra at various distances from excitation spot was performed. We show that photon recycling takes place in thin MAPI films, while its efficiency strongly depends on film morphology defined by preparation approach. Additionally, we discuss here the observed light-soaking effects.

CPP 48.7 Wed 17:00 C 130

Transient Photoluminescence Studies of $CH_3NH_3PbI_3/PC_{61}BM$ Heterojunctions — •Benedikt Krogmeier[1], Florian Staub[1], David Grabowski[1], Uwe Rau[1], and Thomas Kirchartz[1,2] — [1]IEK5-Photovoltaik, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Faculty of Engineering and CENIDE, University of Duisburg-Essen, Carl-Benz-Str. 199, 47057 Duisburg, Germany

Lead-halide perovskites have shown long bulk lifetimes in thin film photovoltaics, which implies that devices are limited by the interfaces and that studying the selectivity of contacts can lead to further improvement. One method proposed for obtaining interface properties is studying the transient photoluminescence of a lead-halide perovskite and an electron- or hole-transfer material layer. Previous studies analyze the photoluminescence transients using either rate equations or analytical solutions to the diffusion equation and do not take nonlinearities caused by charge accumulation at the interface into account. Therefore we use numerical drift-diffusion simulations of the transient photoluminescence of $CH_3NH_3PbI_3/PC_{61}BM$ heterojunctions which enables us to study the impact of laser fluence and interface properties without neglecting the non-linearities. The results show that charge accumulation can have a major impact on the lifetime measured with transient photoluminescence. Comparing simulated photoluminescence with measured data gives us insight into the dominating charge carrier loss mechanisms at different laser fluences and an analysis of the uniqueness of our result enables us to obtain an interfacial recombination velocity of 200 cm/s.

CPP 48.8 Wed 17:15 C 130

Tunable Anisotropic Photon Emission from Self-Organized CsPbBr3 Perovskite Nanocrystals — •Thomas Morgenstern[1], Matthew J. Jurow[2], Erika Penzo[2], Jun Kang[2], Matthew A. Koc[3], Thomas Zechel[1], Zachary Nett[2], Michael Brady[2], Lin-

Wang Wang[2], A.Paul Alivisatos[2,3,4], Stefano Cabrini[2], Yi Liu[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States — [3]College of Chemistry, University of California, Berkeley, California 94720, United States — [4]Kavli Energy NanoScience Institute, Berkeley, California 94720, United States

The introduction of preferentially aligned transition dipole moment vectors (TDMVs) is a common concept in the field of organig light emitting diodes. However, in the literature of perovskites and especially CsPbBr$_3$ nanocrystals this effect has rarely been reported.

In this work the anisotropy factor, correlating to the alignment of the transition dipoles within the nanocubes, for several CsPbBr$_3$ nanocrystal systems has been determined. [1] The results indicate a preferential alignment in vertical direction to the underlying surface. Using theoretical predictions the observed effect can be attributed to a charge redistribution originating from the contact of the nanocrystal to its underlying surface. Thus, a suitable choice of the substrate material can be used to further control the anisotropic emission properties, giving further potential to improve emission properties for light emitting devices. [1] M. Jurow, et. al.: *Nano Lett.* **17(7)** (2017), 4534-4540

CPP 48.9 Wed 17:30 C 130

Circular photogalvanic effect in single-crystal (CH$_3$NH$_3$)PbI$_3$ — •Daniel Niesner[1], Martin Hauck[2], Shreetu Shrestha[3], Ievgen Levchuk[3], Gebhard J. Matt[3], Andres Osvet[3], Miroslaw Batentschuk[3], Christoph J. Brabec[3,4], Heiko B. Weber[2], and Thomas Fauster[1] — [1]Lehrstuhl für Festkörperphysik, Univ. of Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]Lehrstuhl für Angewandte Physik, Univ. of Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [3]Institute of Materials for Electronics and Energy Technology (I-MEET), Univ. of Erlangen-Nürnberg, Martensstr. 7, D-91058 Erlangen, Germany — [4]Bavarian Center for Applied Energy Research (ZAE Bayern), Haberstr. 2a, D-91058 Erlangen, Germany

The mechanisms underlying the remarkable phototransport properties of organic-inorganic perovskite compounds (OIPCs), such as carrier diffusion lengths > 1 μm despite the moderate carrier mobilities, remain a matter of ongoing debate. Rashba and Dresselhaus spin-splittings have been predicted to enhance both carrier lifetimes and electron-acoustic-phonon coupling. Spin-splittings at the surface of an OIPC were measured using photoelectron spectroscopy, but little information exists to quantify their occurrence in bulk material. In a system with spin-split bands, the direction of diffusive photocurrents excited with circularly polarized light is reversed when the helicity of the light is changed. The phenomenom is known as the circular photogalvanic effect. We demonstrate this effect in (CH$_3$NH$_3$)PbI$_3$ single-crystal devices and discuss its relationship to optical properties.

CPP 49: Soft Matter Physics: Emerging Topics, New Instruments and Methods

Time: Wednesday 15:00–17:45 Location: C 230

CPP 49.1 Wed 15:00 C 230

Collective Hydration Dynamics in Binary Mixtures: A THz Time Domain Spectroscopic Study — •Debasish Das Mahanta, Dipak Kumar Das, Animesh Patra, Nirnay Samanta, and Rajib Kumar Mitra — S. N. Bose National Centre for Basic Sciences, Block-JD, Sector-III, Saltlake, Kolkata-700106

We have studied the structure and dynamics of water in its binary mixture with two amphiphilic molecules 1,2-dimethoxy ethane (DME) and dimethyl sulfoxide (DMSO) by THz time domain spectroscopy (TTDS) (0.3-1.6 THz region). In both the cases a non-ideal behavior of the mixture is found owing to the formation of water clusters. The cooperative dynamics of water in those binary mixtures, obtained from Debye relaxation of TTDS data reveals a non-monotonous behavior as a function of water concentration (Xw).

CPP 49.2 Wed 15:15 C 230

Initiation of bimolecular ground-state reaction via IR excitation — •Till Stensitzki[1], Yang Yang[1], Valeri Kozich[1], Ashour A. Ahmed[2,3], Florian Kössel[1], Oliver Kühn[3], and Karsten Heyne[1] — [1]Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Faculty of Science, Department of Chemistry, University of Cairo, 12613 Giza, Egyp — [3]Institute of Physics, University of Rostock, Albert Einstein-Strasse 23-24, 18059 Rostock, German

Excitation of vibrations that participate in the reaction coordinate are believed to accelerate an otherwise thermally driven chemical reaction. Here, we demonstrate the acceleration the thermal driven chemical reaction between cyclohexanol and phenylisocyanate in THF. Upon excitation of the OH-stretching vibration of CH-ol we track bleaching signals of PHI and the urethane product band in real-time. Additionally, we determined reaction rate changes upon selective vibrational excitation with negligible heating of the sample and observed an increase of the reaction rate up to 24%. We utilized reaction acceleration between toluene-2,4-diisocyanate and 2,2,2-trichloroethane-1,1-diol to write a polyurethane square on the sample windows by femtosecond IR pulses.

CPP 49.3 Wed 15:30 C 230

New neutron spectrometer NEAT at Helmholtz Zentrum Berlin for investigation of functional dynamics at nanoscale — Gerrit Günther, Veronika Grzimek, and •Margarita Russina — Helmholtz Zentrum Berlin für Materialied und Energie, Hahn-Meitner Platz 1, 14109 Berlin

Neutron time-of-flight spectrometer NEAT has a long history of successful application to the study dynamics and function. It is best suited to probe dynamic phenomena directly in the broad time domain of 0,1-100 ps and on the large length scale ranging from 0.05 to up to about 5 nm. Recent upgrade of the instrument resulted in 300 fold higher count rate compare to predecessor placing NEAT on the level of the world best. The advanced features of the new instrument include novel integrated guide-chopper system which deliver neutron beam with variable characteristics and substantial increase of the detector angle coverage with simultaneous increase of angular resolution. New instrumental capabilities provides optimal experimental conditions for investigation of microscopic dynamics in soft and hard matter including single excitations in crystals, applications with high magnetic field up to 14 T or in-situ confinement of gasses and liquids in porous systems. Here we present details of NEAT upgrade, measured instrument characteristics and show first experimental results.

CPP 49.4 Wed 15:45 C 230

Second-Harmonic Scattering: Theory and Atomistic Simulation — •David M. Wilkins[1], Sylvie Roke[2], and Michele Ceriotti[1] — [1]Laboratory of Computational Science and Modeling, IMX, EPFL, Lausanne, Switzerland — [2]Laboratory for fundamental BioPhotonics, Institutes of Bioengineering and Materials Science and Engineering, School of Engineering, and Lausanne Centre for Ultrafast Science, EPFL, Lausanne, Switzerland

Recent second-harmonic scattering (SHS) experiments on electrolyte solutions have shown evidence of long-ranged ion-induced intermolecular correlations between solvent molecules, persisting on the $\sim$10 nm length scale at sub-molar concentrations. SHS is exquisitely sensitive to these subtle structural changes, and an atomistic understanding of the kinds of correlations probed is desirable.

I discuss the development of a computational framework for modelling SHS experiments of general condensed-phase systems. This includes two main ingredients: firstly, the orientational correlations between molecules, and secondly, the molecular hyperpolarizability tensor. I show that, at variance with common assumptions, even in an isotropic liquid the modelling of the SHS signal requires that correlations be accounted for, and that the hyperpolarizability tensor depends strongly on the molecular environment. Further, I discuss a machine-learning framework we have developed to sidestep computationally expensive calculations of this tensor, which provides a large step towards the routine calculation of SHS intensities of general systems using machine-learning methods.

CPP 49.5 Wed 16:00 C 230

Symmetry-Adapted Machine-Learning for Tensorial Properties of Atomistic Systems — •Andrea Grisafi, David Mark Wilkins, and Michele Ceriotti — Laboratory of Computational

Science and Modeling, EPFL, Lausanne, Switzerland

In the last few years, machine-learning methods have played a prominent role in providing an accurate description of atomic-scale properties, bypassing computationally demanding quantum chemistry calculations.

A great deal of effort has been applied to learning the ab initio ground state energy of materials and molecules, giving accurate potential energy surfaces. However, a complete description of a condensed phase system requires the calculation of properties that are tensorial in nature, e.g., multipole moments. Unlike scalar quantities, these properties transform in prescribed ways when the reference frame is rotated, presenting a great challenge when designing a machine-learning algorithm.

I discuss an extension of a traditional machine-learning method which can be used to predict tensorial properties of arbitrary rank for systems of arbitrary complexity, automatically encoding the rotational symmetry in three dimension. The novel algorithm has the potential to cover a broad range of applications within material science and condensed matter physics. Applications are shown for the prediction of the electrical response series of water oligomers, from the single molecule to the condensed-phase. Preliminary results for the prediction of the ab initio charge density of organic molecules will be also presented.

CPP 49.6 Wed 16:15 C 230

A generalized convex hull construction for computational materials discovery — •Andrea Anelli, Edgar Engel, and Michele Ceriotti — EPFL, Lausanne,Switzerland

Computational materials searches have the ultimate goal of discovering technologically relevant materials with desired physical properties. State of the art methods can generate thousands of locally-stable configurations. Selecting among these the few structures that can be experimentally synthesised is a needle-in-a-haystack kind of problem.

Conventionally, this screening is performed using a convex hull construction (CH), which can only identify structures stabilized by manipulation of a particular thermodynamic constraint (e.g. density or composition) chosen on the basis of experimental evidence or intuition.

The predictive power of such a formulation is weakened by its dependence on prior knowledge of the system, disregarding configurations that could appear as (meta-)stable under unconventional choices of constraints. We introduce a generalized CH based on an abstract representation of structural features, which are dependent solely on the cartesian coordinates of the systems and constitute a general, agnostic set of thermodynamic constraints. We further introduce a probabilistic scheme that is consistent with uncertainty quantification of the convex-hull construction, reducing the impact of modelling errors on the determination of synthesizable structures. We demonstrate the predictive power of our formulation by applying it to Hydrogen at TPa pressures, the binary high-pressure Oxygen-Hydrogen system and, increasing the structural complexity of the system, on Pentacene molecular crystals

15 min. break

CPP 49.7 Wed 16:45 C 230

In-situ characterization of NiFeOOH for the oxygen evolution reaction using X-ray absorption spectroscopy — •Dorian Drevon — Albert-Einstein-Strasse 15, Berlin

Reducing global carbon emissions will require efficient catalysts for use in solar-to-fuel conversion processes, where electrochemical water oxidation is the key to a zero emission cycle. For this, understanding the fundamental processes of the oxygen evolution reaction (OER, $4OH^- * O_2 + 2H_2O + 4e^-$) from a mechanistic perspective is an important goal for the design of highly efficient and functional electrocatalysts.

The Ni-Fe oxyhydroxide electrocatalysts are currently the most active OER catalysts in alkaline media Combining Ni and Fe leads to an excessive increase in the catalytic activity and a coincident change at the metal redox states, witnessing of the electronic interaction between Ni and Fe sites. However, the complexity of the metal redox activity have resulted in a debate regarding the OER active state in this electrocatalyst.

In-situ O K-edge X-ray and Fe,Ni L-edge absorption fine structure (XAFS) spectroscopy was used to investigate the electronic and structural change in the Nickel Iron electrocatalyst during the oxygen evolution reaction (OER). Above 0.5V versus Ag/AgCl, we were able to see the rise of pre-features at the Oxygen k-edge and post feature at the Nickel L-edge but they were absent in the Fe L-edge suggesting that Ni undergoes a change in its oxidation state from Ni(II) to of Ni(III,IV) when the catalysts becomes active.

CPP 49.8 Wed 17:00 C 230

In-situ R-SoXS study of the structure formation during solvent annealing in organic thin films for application in photovoltaics — •Mihael Coric[1], Isvar Cordova[2], Gregory Su[2], Feng Liu[3], Cheng Wang[2], and Eva M. Herzig[1,4] — [1]TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, 94720 Berkeley, USA — [3]Department of Physics and Astronomy, Shanghai Jiaotong University, 200240 Shanghai, China — [4]Universität Bayreuth, Physikalisches Institut, Herzig Group - Dynamik und Strukturbildung, 95440 Bayreuth, Germany

Resonant X-ray scattering (R-SoXS) at the carbon edge is now an established, very powerful tool for the analysis of structure and morphology formation in organic thin films. Since soft X-rays have a very low penetration depth and strong air scattering, samples need to be measured in high vacuum, but offer a much higher contrast than hard X-rays. However, in regards to the examination of structure formation, in-situ studies are essential to achieve a better understanding of the formation processes taking place in thin films. In this work, we present a method using the well-known R-SoXS technology with a setup that enables us to execute in-situ studies under a steady flow of vapor inside the vacuum chamber. We will show that it is possible to track changes in the morphology of organic thin film materials during a solvent annealing process. In combination with in-situ UV-Vis measurements, we are able to gain a better understanding of the structure and formation processes involved.

CPP 49.9 Wed 17:15 C 230

EMIL goes operando: *In-situ* characterization of real-world electrocatalysts by soft x-ray spectroscopy — •Raul Garcia-Diez[1], Regan G. Wilks[1,2], and Marcus Bär[1,2] — [1]Renewable Energy, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), Berlin (Germany) — [2]Energy Materials In-Situ Laboratory Berlin (EMIL), HZB, Berlin (Germany)

The *in-situ* study of catalyst materials during the electrolysis of water is of vital importance to understand the limiting mechanisms occurring in the catalytic reaction. The combination of soft x-ray absorption (XAS) and emission (XES) spectroscopies is an established method that can probe the chemical and electronic structure of the electrocatalyst and give insights into its local density of states and, therefore, its catalytic behavior.

For this purpose, in the Energy Materials In-Situ Laboratory Berlin (EMIL) at the BESSY II synchrotron facility we are developing an infrastructure that allows XAS, XES, and RIXS (resonant inelastic x-ray scattering) *operando* studies based on a 3-electrode electrochemistry flow-cell located at the HZB's branch of the EMIL beamline. The modular design of the measurement chamber ensures an easy connection to the newly developed high-transmission soft x-ray emission spectrometer, which covers the photon range between the Li and the Si K-edge with an energy resolving power > 1500.

We present the current status of the instrumentation in EMIL and the first spectroscopic results on our path towards the *in-situ* characterization of real-world electrocatalysts under operating conditions.

CPP 49.10 Wed 17:30 C 230

Lab-on-a-chip - Electron paramagnetic resonance goes mini — •Silvio Künstner[1], Benedikt Schlecker[2], Anh Chu[3], Jannik Möser[1], Alexander Schnegg[1], Jens Anders[3], and Klaus Lips[1] — [1]Berlin Joint EPR Laboratory, Helmholtz-Zentrum Berlin für Materialien und Energie — [2]Insitut für Mikroelektronik, Universität Ulm — [3]Institut für Theorie der Elektrotechnik, Universität Stuttgart

Electron paramagnetic resonance (EPR) spectroscopy is one of the most powerful techniques used in physics, chemistry and materials science. It is a non-invasive technique sensitive to paramagnetic species, especially suited for the study of paramagnetic states in thin-film materials and at surfaces involved in chemical reactions. However, the current design of EPR spectrometers using a microwave (mw) resonator limits the versatility for operando measurements. Here, we present a radical new design of a miniaturised EPR spectrometer, implemented on a microchip (EPR-on-a-chip). EPRoC is no longer restricted by the boundary condition of a resonator and has a three order of magnitude higher spin sensitivity than conventional EPR. The sensor is a single coil scaled-down in size to a few 10-100 micrometer. Different from conventional EPR, EPRoC is carried out by sweeping the mw frequency instead of the magnetic field, enabling operation with a permanent magnet. Due to its compactness, EPRoC can be incorporated in conventional growth reactors, (electro)chemical cells or in harsh UHV environments. We will review the recent success of operando EPRoC, discuss the detection principle and demonstrate its superior sensitivity, and present first time-domain experiments with nanosecond resolution.

CPP 50: Charged Soft Matter, Polyelectrolytes and Ionic Liquids II

Time: Wednesday 15:00–17:15 Location: C 243

CPP 50.1 Wed 15:00 C 243

Polyelectrolyte Complexes with Oppositely Charged Microemulsion Droplets: Investigations of Structure and Dynamics — •Michael Gradzielski[1], Miriam Simon[1], Laurence Noirez[2], and Ingo Hoffmann[3] — [1]Stranski-Laboratorium, Institut für Chemie, TU Berlin — [2]Laboratoire Leon-Brillouin (LLB), Saclay, France — [3]Institut Laue-Langevin (ILL), Grenoble, France

Mixing polyelectrolytes (PE) with oppositely charged colloids leads to modifications of structure and rheology of the systems. For the case of surfactants that leads to polyelectrolyte/surfactant complexes (PESCs). As loaded micelles are relevant for delivery we studied mixtures of positively charged O/W microemulsion (ME) droplets with negatively charged polyelectrolytes. Based on a thorough determination of the phase behavior, the combination of SLS, DLS, SANS yielded a detailed description of the formed complexes in terms of size, shape and composition. Dynamics were studied by PFGNMR, NSE, and FCS. This yielded a comprehensive picture of how the structure depends on ME size and the type and Mw of the PE.

CPP 50.2 Wed 15:15 C 243

Electronic Continuum Correction for Multivalent Ions in Water — •Ellen Bruce and Nico van der Vegt — Technische Universität Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt, Germany

Short range interactions between hydrated ions and/or charged chemical groups on (bio)polymers lie at the basis of several physical phenomena in aqueous solvation science that remain ill-understood. These interactions are commonly studied with molecular simulation methods that use non-polarizable models, as these are computationally cheap. This approach is however problematic due to strong electronic polarization effects. One way of accounting for polarization effects in non-polarizable models is by using the electronic continuum correction (ECC).[1] ECC has been widely used for monovalent and some divalent salts. However, the performance for multivalent salts which have stronger polarization effects is largely unexamined. We show that the ECC model provides accurate description for multivalent ions solutions (K3PO4 and K2HPO4).[2] The osmotic coefficients are used as a measure to assess ECC models and are in good agreement with experiments. The results demonstrate accurate modeling of electrolyte structure as well as effective short-range ion-ion interactions. This approach opens routes for simulations of aqueous soft matter systems in which short-range electrostatic interactions drive interesting physical phenomena. [1] I. V. Leontyev et al., J. Chem. Phys. 119, 8024 (2003) [2] E. E. Bruce et al., J. Chem. Phys. (submitted 2017)

CPP 50.3 Wed 15:30 C 243

Solvate induced surface order in ionic liquids — •Julian Mars[1,2], Henning Weiss[2], Sven Festersen[3], Bridget Murphy[3], Veijo Honkimäki[4], Markus Bier[5], and Markus Mezger[1,2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institute of Physics and MAINZ Graduate School, Johannes Gutenberg University Mainz, Germany — [3]Institute of Experimental and Applied Physics, Kiel University, Germany — [4]ESRF The European Synchrotron, Grenoble, France — [5]Max Planck Institute for Intelligent Systems, Stuttgart, Germany

In supported ionic liquid (IL) phase catalysis, the chemical reaction takes place in a sub-micrometer IL film, wetting a solid support material with high surface area. To understand diffusion of reactants and products across the IL/vapor interface, knowledge of the interfacial structure is crucial. We employ X-ray scattering techniques to investigate the near surface structure on the molecular length scale. In microheterogeneous ILs, solvates aggregates site-specifically within high affinity domains. Non-polar molecules are preferentially situated in the aliphatic regions, affecting the near surface structure. For different classes of binary model systems, we observe the formation of adsorbate layers and solvate induced surface phase transitions.

CPP 50.4 Wed 15:45 C 243

Effect of Salt on the Surface Absorption and Structures of aqueous Polyelectrolyte/Surfactant Mixtures at the air/water Interface — •Larissa Braun[1], Richard Campbell[2], and Regine von Klitzing[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]Institut Laue-Langevin, Grenoble, France

The surface properties of mixtures of polyelectrolyte and oppositely charged surfactant play an important role in colloidal dispersions (foams, emulsions) e.g. for cosmetics, cleaning products and in food technology.

This work focuses on the effect of salt (LiBr) on the adsorption behavior of mixtures of the anionic polyelectrolyte sPSO2-S220 with the cationic C14TAB. Neutron reflectometry experiments including extensive contrast matching were performed to get insight into the exact composition and structure of the adsorbed polyelectrolyte/surfactant complexes at the air/water interface.

There is no linear relation between surface composition and bulk composition. The salt influences both the surface composition as well as the formed structures at the surface.

CPP 50.5 Wed 16:00 C 243

Counterions in aqueous planar nano-confinement: Atomistic simulations and continuum modeling — •Alexander Schlaich[1,2] and Roland R. Netz[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Laboratoire Interdisciplinaire de Physique (LIPhy), CNRS and Université Grenoble Alpes, F-38000 Grenoble, France

Continuum models for the electrostatic interaction between charged surfaces have been employed successfully to model the interaction between charged surfactants and lipid membranes, yet in nanoconfinement additional effects such as the hydration force and dielectric effects need to be taken into account. Here, we perform water-explicit atomistic simulations of monovalent counter-ions confined between planar, charged decanol surfaces at prescribed water chemical potential, allowing to access the interaction pressures and charge distributions in sub-nanometer confinement. At low surface charge density we find additive contributions to the repulsion due to the exponential hydration interaction and counterion entropic effects. The modified Poisson-Boltzmann equation, including the dielectric profile, the fluctuating external charge distribution of the surface and ion-surface interactions, quantitatively describes the ion distribution from several nanometer separations down to strongest confinement, corresponding to kilobar interaction pressures.

CPP 50.6 Wed 16:15 C 243

Effects of counterions on conformation and counterion condensation on polyelectrolytes — •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str 6, 01069 Dresden, Germany

Counterion condensation reduces the effective charge in polyelectrolytes. This in turn affects the conformation of the polyelectrolytes, because the repelling force between repeat units is reduced. The hydrodynamic size of the polyelectrolytes in solution is determined from the selfdiffusion coefficient measured by PFG NMR. In combination with electrophoresis NMR the effective charge is determined and compared with the nominal charge from the number of repeat units. Poly(styrenesulfonate) has been titrated with various hydroxides to generate the respective salts. There are the expected differences between mono and bivalent counterions, with the latter resulting in an effective charge reduced by about a factor of two and a hydrodynamic radius reduced by 30%. However the effective charge of the acid with H+ as counterion is 10% larger than for others monovalent counterions. Significant differences in the hydrodynamic radius are observed, which are not simply explained by the counterion condensation. Ion-specific effects are observed as well.

15 min. break

CPP 50.7 Wed 16:45 C 243

Temperature dependence and thermal response of electric double layer capacitors — •Mathijs Janssen — Max Planck Institute for Intelligent Systems, Stuttgart, Germany

Where surfaces of charged electrodes meet fluids that contain mobile ions, so-called electric double layers (EDLs) form to screen the electric surface charge by a diffuse cloud of counterionic charge.

In this talk, we discuss the intricate interplay between temperature and EDL characteristics. First, we show that varying the electrolyte temperature gives rise to a temperature-induced surface charge variation [1]. Vice versa, variation of the electrode potential of a thermally insulated EDL capacitor gives rise to a charge-induced temperature variation [2]. Besides irreversible (bulk) Joule heating, this temperature variation is sourced by the reversible ion rearrangements that occur during EDL formation: heating upon charging, and cooling upon discharging. We derive a thermodynamic identity for this isentropic-heating-by-charging effect, and compare to the slow-charging thermal behavior of a Nernst-Planck model [2]. We finally argue that the thermal response to charging in fact contains valuable information on the EDL; we deduce the entropic part of the grand potential from the tiny temperature variations that can be measured during charging and discharging an EDL capacitor [3].

[1] M. Janssen et al., Phys. Rev. Lett. 113, 268501 (2014)

[2] M. Janssen and R. van Roij, Phys. Rev. Lett. 118, 096001 (2017)

[3] M. Janssen et al., Phys. Rev. Lett. 119, 166002 (2017)

CPP 50.8 Wed 17:00 C 243

A computational study on the properties of residual water in ionic liquids using the Kirkwood-Buff theory — •Takeshi Kobayashi[1], Joshua E. S. J. Reid[2,3], Seishi Shimizu[2], Maria Fyta[1], and Jens Smiatek[1] — [1]Institute for Computational Physics, Universität Stuttgart, Germany — [2]York Structural Biology Laboratory, Department of Chemistry, University of York, UK — [3]TWI Ltd., UK

The properties of residual water in two different dialkylimidazolium based ionic liquids (ILs), namely 1-ethyl-3-methylimidazolium tetrafluoroborate (EMIM/BF4) and 1-butyl-3-methylimidazolium tetrafluoroborate (BMIM/BF4), are studied at different water mole fractions by means of classical atomistic molecular dynamics simulations[1]. In order to provide a robust validation of the simulation results, the Kirkwood-Buff (KB) integrals for the ion-ion and ion-water pair correlations are calculated from the corresponding radial distribution functions and compared with the inverse KB results based on experimental data. It is shown that there is a quantitative agreement between these two approaches. Further analysis shows a negligible influence of residual water on the structures of ILs even at intermediate mole fractions. The majority of the water molecules are found as monomers, while a non-linear increase in the higher order water clusters is observed for higher mole fractions. According to these results, our work provides a detailed explanation of the properties of the binary mixtures of water and dialkylimidazolium based ILs. [1] T. Kobayashi et al., Phys. Chem. Chem. Phys. 19, 18924 (2017)

CPP 51: Hydrogels and Microgels

Time: Wednesday 15:00–17:00 Location: C 264

CPP 51.1 Wed 15:00 C 264

On the generation of stimuli-responsive HEMA-co-DEAEMA hydrogels by using Cold Atmospheric-Pressure Plasma Polymerization — •Ihsan Amin[1], Felipe Vicente de Paula Kodaira[1,2], Monique Levien[1], Rogério Pinto Mota[2], Klaus-Dieter Weltmann[1], and Katja Fricke[1] — [1]Junior Research Group Biosensing Surfaces, Leibniz Institute for Plasma Science and Technology, INP Greifswald e.V., Felix-Hausdorff-Strasse 2, 17489 Gerifswald, Germany — [2]São Paulo State University (Unesp), School of engineering, Guaratinguetá, SP, Brazil

A simple and fast fabrication of stimuli-responsive hydrogels from (hydroxyethyl)methacrylate-co-2-(diethylamino)ethyl methacrylate by cold atmospheric plasma polymerization (CAPP) is reported. The influence of input power and different volume ratios on the coating's properties have been investigated to clarify their effect on the stability and swelling behavior of the hydrogels. The plasma-polymerized hydrogels retain the functionality of both monomers and their functional groups, as measured by FTIR and XPS. Hydrogel films generated at a HEMA/DEAEMA volume ratio of 1:1 demonstrate good stability and a high swelling ratio in water at pH 7, and a lower swelling ratio at pH 10 and pH 4, respectively. Due to the simplicity and cost efficiency of CAPP, combined with the excellent properties of the plasma polymerized hydrogels, these coatings are suitable for biomedical applications such as biosensors, implants, and cell adhesion-promoted coatings where long-term stability of the surface properties is required.

CPP 51.2 Wed 15:15 C 264

Foams stabilized by PNIPAM microgels — •Matthias Kühnhammer and Regine von Klitzing — Technical University of Darmstadt, Department of Physics, Soft Matter at Interfaces, 64287 Darmstadt, Germany

Cross-linked, short-chained poly-N-isopropylacrylamide (NIPAM) polymers, also referred to as microgels, have attracted much attention during the last years and were studied with various techniques and in the context of multiple possible applications. Since these microgels are responsive to external stimuli like temperature, materials made from them can be considered 'smart' materials. A prominent example are thermo-responsive emulsions stabilized by microgel particles adsorbed at the water-oil interface. In these systems the emulsion stability can be controlled by changing the temperature [1,2].

In this contribution we report on our experiments with aqueous foams, which are stabilized by PNIPAM microgel particles. We present how microgel properties like size, cross-linking density and particle concentration can influence properties of macroscopic foams prepared with them. In addition we attempt to link the differences in foamability and foam stability to the properties of the different microgels in solution. [1] B. Brugger, B. Rosen, W. Richtering, Langmuir, (2008), p. 12202. [2] V. Schmitt, V. Ravaine, Curr. Opin.Colloid Interface Sci. (2013), p. 532.

CPP 51.3 Wed 15:30 C 264

Studying properties of microgels: from fuzzy to core-shell model — •Elena Minina[1,2], Sofia Kantorovich[1,2], and Christos Likos[1] — [1]University of Vienna, Vienna, Austria — [2]Ural Federal University, Ekaterinburg, Russian Federation

Microgels are spherical colloidal particles consisting of the polymer network. Due to their nature, microgels are able to swell and shrink as a response to their external environment. This ability makes them promising materials for many applications including drug delivery and design of artificial muscles. The desire to control microgels, therefore, has motivated studying their properties.

In this work, we study microgels properties by means of molecular dynamics computer simulations. To this aim, we developed coarse-grained models of fuzzy and core-shell microgels based on the bead-spring model and random cross-linking procedure. Our models capture the swelling behaviour of microgels that we verified by embedding microgels in solvents of different quality. To examine structural properties of microgels, we focus on the polymer network analysis and density profiles of microgels of different size and with various fraction of homogeneously distributed cross-linkers inside the core and on the shell for core-shell microgels.

CPP 51.4 Wed 15:45 C 264

Anomalous Dynamics of Concentrated Silica-PNIPAm Microgels — •Lara Frenzel[1,2], Felix Lehmkühler[1,2], Irina Lokteva[1,2], Michael Sprung[1], and Gerhard Grübel[1,2] — [1]DESY, Notkestr. 85, 22607 Hamburg — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg

Poly(N-isopropylacrylamide) (PNIPAm) cross-linked microgels show a coil-to-globule transition in water at a lower critical solution temperature (LCST) around 32°C, below which the particles collapse drastically. With this volume phase transition PNIPAm is applicable in both technical as well as medical fields. It furthermore became a frequently studied system in soft matter research as a model system to probe the specific phase behavior of soft colloids. Via x-ray photon correlation spectroscopy (XPCS) we investigate the change of structure and dynamics of highly concentrated PNIPAm core-shell microgels around the LCST. Here we will present our work on particles with radii of 80-200 nm, whereby we investigated the dynamics and interaction of the highly concentrated colloids as a function of temperature. Upon heating from room temperature to 45°C we found three dynamical regimes: First, the relaxation time decreases linearly while the shell shrinks. Second, around the LCST at 32°C the relaxation time decreases rapidly until it (third) jumps around 38°C more than three orders of magnitude. This effect was determined as a function of concentration between 6 and 30 wt% and is not present in dilute systems. Furthermore, both the structural and the dynamical behavior were found to be reversible upon cooling down the system after heating.

CPP 51.5 Wed 16:00 C 264

Combining reaction ensemble Monte-Carlo simulations with Molecular Dynamics to probe the electrophoretic mobility of weak polyelectrolytes — •David Sean and Christian Holm — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

Monomers in strong polyacids become negatively charged due to a strong chemical drive bringing them towards a deprotonated state. In weak polyelectrolytes however, the chemical drive is weak and monomer ionization often change between its (negatively charged) dissociated state and a (neutral) associated state. The reaction ensemble Monte-Carlo (RxMC) method allows to efficiently sample configurational states of weak polyelectrolytes under chemical equilibrium in order to obtain static properties. However, this method is inappropriate probe dynamical properties like diffusion and electrophoretic mobility. In order to probe for dynamical properties, we turn to Molecular Dynamics (MD) with hydrodynamic interactions using the Lattice Boltzmann method. With the chemical equilibrium results obtained from the RxMC simulations, MD simulations are used to integrate in time the trajectories polyelectrolytes under the influence of a driving field. Static and dynamic properties of a coarse-grained microgel model in salty conditions are reported using this methodology. We report and discuss upon a surprisingly weak dependence of the mobility as a function of the total nanogel charge.

CPP 51.6 Wed 16:15 C 264

Modelling of shock wave dynamics in ferrogels — •Segun Goh, Andreas M. Menzel, and Hartmut Löwen — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany

Ferrogels are smart soft materials, consisting of a gel network and embedded magnetic particles. Novel phenomena, such as the response of elasticity to external magnetic fields, emerge consequently. Due to the difficulties in describing the touching/separating processes of magnetic particles, however, the dynamics of ferrogels remain largely unveiled. In this study, we consider a one dimensional chain consisting of magnetic dipoles and springs between them as a simple model for ferrogels. To probe the dynamics theoretically, we investigate a continuum limit of the double-well type potential governing the system and the corresponding equation of motion. It is then revealed that a type of spinodal decomposition underlies the touching/separating dynamics of the magnetic particles. We further elucidate the formation of touching/separating particle clusters as well as the migration of interfaces in terms of shock solutions. Comparisons of the continuum theory with the particle-resolved simulation are also given. We expect that these results will provide insight into understanding the dynamics of more realistic models with randomness in parameters and time-dependent magnetic fields.

15 min. break

CPP 51.7 Wed 16:45 C 264

Alternative acrylamides for microgel synthesis — •Yvonne Hertle[1], Jörn Lessmeier[1], Johanna Grote[2], Lars Wiehemeier[1], Tilman Kottke[1], Sergej Kakorin[1], and Thomas Hellweg[1] — [1]Physical and Biophysical Chemistry, Bielefeld University, Bielefeld, Germany — [2]Inorganic and Structural Chemistry, University Bielefeld, Bielefeld, Germany

Microgels made of poly(N-isoproplyacrylamide) (pNiPAM) are one of the most frequently used and studied polymer based systems in the field of soft matter. Due the LCST (lower critical solution temperature) of pNiPAM in water at about 32°C, microgels made of this polymer are suitable candidates for a wide variety of applications like nanoparticle and drug carriers, sensors, nanoactuators, chemical separation media or biochemical applications as cell culture media.

Since the monomer NiPAM and its relative N-isoproplymethacrylamide (NiPMAM) are commercially available, other homologous acrylamides need to be synthesized. Therefore, the Schotten-Baumann reaction published by Hirano et al. for the synthesis of N-n-propylacylamide (NnPAM) is well suited [1]. Based on this we established a synthesis route to obtain a wide variety of acrylamide monomers. From these homopolymer microgels and different copolymer particles have then been prepared via a conventional precipitation polymerization with surfactant and characterized with respect to their phase transition behaviour, particle size and composition.

[1] B. Wedel, Y. Hertle, O. Wrede, J. Bookhold and T. Hellweg, Polymers, 8, 2016, 162.

CPP 52: Bioinspired Functional Materials, Biomaterials and Biopolymers (joint session CPP/BP)

Time: Wednesday 15:00–16:30 Location: PC 203

CPP 52.1 Wed 15:00 PC 203

Specific Ion Effects of Protein-Coated Au NPs: The Influence of Hydroxide Formation on Charge and Stability — •Jonas Schubert[1,2], Andreas Fery[1,2], and Munish Chanana[3,4] — [1]Department of Nanostructured Materials, Leibniz-Institut für Polymerforschung Dresden e. V. — [2]Physical Chemistry of Polymer Materials, Technische Universita*t Dresden, D-01062 Dresden, Germany — [3]Institute of Building Materials (IfB), ETH Zurich, 8093 Zurich, Switzerland — [4]EMPA Dübendorf, 8600, Dübendorf, Switzerland.

When NPs are exposed to the environment, a protein corona is generated around the NPs. This changes the physicochemical properties of the NPs drastically, especially their colloidal stability, which is a key feature for discovering their bioavailability, toxicity and fate in the environment. In this work, the impact of the type of protein corona on the colloidal stability towards different ions was investigated by using three different proteins. Au NPs were coated with bovine serum albumin, beta-lactoglobulin and insulin and tested against different ions. The particles exhibited a highly pronounced and dissimilar optical response towards various heavy metal ions. The response of the Au@Protein NPs towards the different metal ions strongly depends on the protein coating of the NPs, but also on the specific metal ion and the generation of metal hydroxides. We discovered that the generation of metal hydroxides is the determining factor for the dissimilar colloidal stability of Au@Protein NPs and therefore plays an important and up to now neglected role in the interpretation of specific ion effects.

CPP 52.2 Wed 15:15 PC 203

Denaturation-Induced Fiber Formation of Fibrinogen Studied by Small Angle Scattering — Matthias M.L. Arras[1], •Christian Helbing[2], Klaus D. Jandt[2], and Gregory S. Smith[1] — [1]Oak Ridge National Lab, Oak Ridge, USA — [2]Friedrich Schiller University Jena, Germany

Over the last years, the interest in materials consisting of biomolecules arranged in nanofibers increased. To get a better understanding of how different environmental parameters affect the fiber formation in solution, we studied the ethanol induced fiber formation of human plasma fibrinogen (HPF) by small angle scattering, i.e., (ultra)small angle neutron scattering and light scattering. To this end, we used water/deuterium oxide and ethanol-d6 contrast matched at the scattering length density of ethanol-d6 and varied the protein concentration, as well as ethanol concentration. We find the ethanol-to-water ratio to be a dominant driving force for inducing long fiber formation. Data suggest a 1.5:1 water:ethanol ratio as a threshold, where increasing the water ratio prevents long-fiber formation after an hour of incubation. Time series show, that structure on the protein size-level does not change over time, however the growth in fiber length can still be observed hours after ethanol addition.

This research used resources at the High Flux Isotope Reactor and Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

CPP 52.3 Wed 15:30 PC 203

Direct Determination of the Thermodynamic Properties of Melting for Amino Acids — •Y.Z. Chua[1], A. Abdelaziz[1,2], D. Zaitsau[2], S. Verevkin[2], C. Held[3], and C. Schick[1] — [1]Uni Rostock, Institut für Physik and Competence Centre CALOR, Rostock — [2]Uni Rostock, Institut für Chemie, Rostock — [3]TU Dortmund, Department of Biochemical and Chemical Engineering, Dortmund

The properties of melting are used for the prediction of solubility of solid compounds. By using conventional DSC or adiabatic calorimetry, direct determination of the melting temperature, T_{fus}, and enthalpy of fusion, $\Delta_{\text{fus}}H$, is often not possible for biological compounds due to the decomposition during the measurement. The apparent activation energy of decomposition is at least one order of magnitude smaller than that of melting. This allows shifting of the decomposition process to higher temperature without seriously disturbing the melting by applying very high heating rates. High scanning rates up to $2 \cdot 10^4$ $\text{K}\cdot\text{s}^{-1}$ are utilized with fast-scanning calorimeter Mettler Toledo Flash DSC1. The melting parameters, e.g. T_{fus} and $\Delta_{\text{fus}}H$, for L-threonine and glycine were successfully determined. The ultra-fast cooling of the melted samples allows the studied compounds to retain in the liquid state and to determine for the first time its glass transition temperatures, T_{g}, which agree with the Beaman-Kauzmann rule ($T_{\text{g}} \approx 2/3 \cdot T_{\text{fus}}$). The entropy of fusion shows significant deviation between the two amino acids. For L-threonine, it was close to the Walden's rule, while for glycine, it was twice smaller. The results are in reasonable agreement with the simulated PC-SAFT values.

CPP 52.4 Wed 15:45 PC 203

Cellulose-Based Photoresist for Two-Photon Lithography — •Marie-Christin Angermann[1], Maximilian Rothammer[2], Cordt Zollfrank[2], and Georg von Freymann[1,3] — [1]Physics Department and Research Center OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Chair of Biogenic Polymers, TU Munich, Campus Straubing of Biotechnology and Sustainability, 94315 Straubing, Germany — [3]Fraunhofer Institute for Industrial Mathematics ITWM, 67663 Kaiserslautern, Germany

Lithography is a common method for structuring which uses photoresists based on polymers extracted from mineral oil. To conserve resources those polymers could be replaced by sustainable materials like polysaccharides. So far, no polysaccharide based photoresist has been presented. We here present such a resist by using functionalized cellulose which can be photo-crosslinked by a photoinitiator. For this cellulose and initiator are dissolved in acetone. The resist is curable with two-photon absorption (780 nm) in a direct laser writing system (DLW), and via one-photon absorption with a UV lamp (365 nm), in liquid state as well as in dried state, after evaporation of the acetone. Using DLW and a liquid resist a resolution of 1.6 μm with a feature size of 600 nm is achieved. Furthermore, it is possible to fabricate three dimensional structures. The threshold for polymerization with the DLW depends on the amount of initiator and the amount of acetone influences mainly the durability of the resist.

This resist opens up a new class of photoresist based on sustainable materials.

CPP 52.5 Wed 16:00 PC 203

Atomic force microscopy (AFM) based method to investigate the transversal viscoelastic properties of paper fibers — •Caterina Czibula[1,3], Christian Ganser[1,3], Ulrich Hirn[2,3], and Christian Teichert[1,3] — [1]Institute of Physics, Montanuniversitaet Leoben, Austria — [2]Institute for Paper, Pulp and Fiber Technology, Graz University of Technology, Austria — [3]Christian Doppler Laboratory for Fiber Swelling and Paper Performance, Austria

It is well known that paper fibers are an inhomogeneous and hierarchical material. Resulting structure-property relations on the fiber scale as well as on the paper scale are complicated and not yet fully understood. To gain more insight on how mechanical properties of fibers are related to properties of the paper, our work focusses on the transverse viscoelastic behavior of single pulp fibers. To reach this ambitious goal we implemented an AFM based method.

Probing nanoscale mechanical properties of soft materials with AFM yields information on the performance of the material. Furthermore, precise force control in AFM methods is possible, and with different contact models, the contact between AFM tip and sample surface can be well described. Here, we use the Johnson-Kendall-Roberts model because it includes adhesion. At the continumm scale, simple empiric models combining springs and dash pots are often used to represent the bulk behavior of viscoelastic materials. Here, some of those models are explained and are used to describe local viscoelastic properties on the nanoscale. Results are presented for kraft pulp and compared to those of viscose fibers which are a simpler model system.

CPP 52.6 Wed 16:15 PC 203

Self-consistent Hubbard-corrected DFT study of hole-polaron trapping in glucose-based bio-insulators: the Cyclodextrin case. — •Stefano Mensa and Gilberto Teobaldi — Stephenson Institute for Renewable Energy, Department of Chemistry, University of Liverpool, L69 3BX Liverpool, United Kingdom

Using CyDs as an archetypal glucose-based bio-insulator, we use a self-consistent linear response DFT+U approach, as implemented in the linear-scaling ONETEP code, to explore hole-polaron relaxation both in vacuo and in the presence of different acidic, alkaline and ionic environments due to interacting H(+), OH(-), Na(+) and Cl(-) ions. Hole-polaron trapping in isolated CyDs or in CyDs interacting with H(+), Na(+) and Cl(-) ions is computed to be energetically disfavoured. However, hole-polaron trapping at terminal hydroxyl (-OH) groups becomes energetically favoured by up to -2 eV in the presence of alkaline conditions as a result of hydroxyl deprotonation by interacting OH(-) ions. Selective hole-polaron trapping at glycosidic (C-O-C) bridges between glucose monomers is found to be consistently disfavoured regardless of the presence of interacting ions. The computed stability of the CyD-backbone to direct oxidative depolymerisation, favourable hole-trapping at terminal CyDs hydroxyls, and well known CyDs capability of hosting both organic and inorganic contaminants altogether suggest that CyDs may be effective redox intermediates for the development of novel strategies for photocatalytic oxidation of hosted polluting agents in alkaline conditions.

CPP 53: Solid-liquid interfaces: Reactions and electrochemisty III (joint session O/CPP)

Time: Wednesday 15:00–16:15 Location: MA 144

CPP 53.1 Wed 15:00 MA 144

Atomically-Defined $\text{Pt/Co}_3\text{O}_4(111)$ as Model Electrocatalyst — •Manon Bertram, Corinna Stumm, Firas Faisal, Yaroslava Lykhach, Olaf Brummel, and Jörg Libuda — Physikalische Chemie II, FAU Erlangen

The surface science approach, i.e. studying model catalysts in ultra-high vacuum (UHV), is well known in heterogeneous catalysis. We apply this approach to electrocatalysis and transfer complex, but well-defined catalysts from UHV to electrochemical (EC) conditions.

As a model system we prepared Pt nanoparticles (NPs) on ordered $\text{Co}_3\text{O}_4(111)$ thin films on Ir(100). The oxide support and the complete catalyst were characterized by low-energy electron diffraction (LEED), x-ray photoelectron spectroscopy (XPS) and other methods. We transferred the systems to EC environments under ultra-clean conditions. With a scanning flow cell coupled to an inductively coupled plasma mass spectrometer and EC infrared reflection-absorption spectroscopy (EC-IRRAS), LEED, and XPS we determined the stability window for the oxide support under EC conditions.

Using $\text{Pt/Co}_3\text{O}_4(111)$ with different Pt loadings, we followed the CO electro-oxidation by EC-IRRAS and cyclic voltammetry. As reference, we studied CO adsorption under UHV conditions with infrared reflection absorption spectroscopy. We identify different adsorption sites, a suppression of bridging CO on small NPs, and electronic metal support interactions (EMSI) leading to formation of partially oxidized Pt. The EMSI influences the CO adsorption and, thus, the electrocatalytic properties.

CPP 53.2 Wed 15:15 MA 144

Real-Time Measurement of Silica Dissolution at the interface with water — •Jan Schaefer, Ellen H.G. Backus, and Mischa Bonn — Max Planck Institute for Polymer Research, Mainz, Germany

Dissolution processes of minerals in water are often studied on macroscopic scales by detecting dissolution products in bulk solution and inferring microscopic reaction rates using models that require assumptions. Here, we present a direct way to measure the dissolution rate of silica, a mineral of geological significance, in contact with water. We find that on a surprisingly short timescale of tens of hours, the interfacial concentration of dissolution products saturates at a level close to the solubility of silica (˜ millimolar). As the bulk solution is known to be equilibrated only after several weeks, our results reveal that the macroscopic dissolution process is limited by diffusion. A comparison with a simple 1D reaction/diffusion model indicates that the diffusion coefficient of dissolved silica decays with progressing dissolution which suggests that the small silicic acid species polymerize next to the silica surface.

CPP 53.3 Wed 15:30 MA 144

Charge transfer across the n-GaP(100) photoanode/electrolyte interface during photoelectrochemical water splitting — •waqas saddique, gerhard lilienkamp, and winfried daum — Institute of Energy Research and Physical Technologies, Technical University Clausthal, Clausthal-Zellerfeld, Germany

A detailed understanding of charge transfer across the electrode/electrolyte interface is required for the development of electrodes for efficient water splitting. We have studied the charge transfer processes across the n-GaP(100) photoanode/electrolyte interface at different photoelectrochemical (PEC) conditions. In a 0.02 M HCl electrolyte, high photoanodic currents from n-GaP(100) photoanodes related to photolytic water splitting were measured at low anodic potentials, these currents diminished at cathodic potentials as well as at high anodic potentials. Nyquist plots obtained from electrochemical impedance spectroscopy (EIS) results were analyzed with two different equivalent electrical circuits (EECs) for the electrode/electrolyte charge transfer pathways. For both EECs, the potential dependence of resistances and constant phase elements were determined from fits to Nyquist plots and then compared with the potential variation of the current in the cyclic voltammogram. XPS measurements revealed that the surface oxide consists mainly of Ga2O3, while small concentrations of GaPO4, P2O5 and metal-like Ga are also detected in the topmost layers. Our results suggest that energetically favorable absorption of hydroxide, persumably at metal-like surface Ga, and their subsequent oxidation at low anodic potentials lead to high currents.

CPP 53.4 Wed 15:45 MA 144

Epitaxial oxides as model electrodes for electrolyzer and fuel cell reactions at room temperature — •Marcel Risch, Julius Scholz, Janis Geppert, Lennart Köhler, Garlef Wartner, and Christian Jooss — Georg-August-Universität Göttingen, Institut für Materialphysik,

Energy carriers based on sustainable hydrogen are highly desirable for storage of intermittent renewable energy. The performance of the required electrolyzer and fuel cell technology could be improved significantly by a fundamental understanding of the basic reaction steps of the oxygen electrodes, which present the current bottleneck for electrocatalysis at room temperature. The chemistry and correlation physics of perovskite oxides can be tuned by chemical substitution to derive property-activity relationships [1]. Epitaxial thin films with optimized composition are very active for both the evolution as well as reduction of oxygen [2]. Moreover, perovskite oxide films of conductive (La,Sr)MnO3 showed terraces with unit cell step height and the perovskite structure was preserved after electrolysis in alkaline solution [3]. These properties make perovskite oxides ideal model surfaces to elucidate the catalytic mechanisms of oxygen evolution and reduction at room temperature. It will be discussed how the combination of materials physics, electrochemistry and spectroscopy leads to the desired mechanistic insight on selected perovskite oxides with defined surfaces.

References: [1] Risch et al., Catalysts 7, 139 (2017); [2] Risch et al., J. Am. Chem. Soc. 136, 5229 (2014); [3] Scholz et al., J. Phys. Chem. C 120, 27746 (2016), Scholz et al., Catalysts 7, 139 (2017).

CPP 53.5 Wed 16:00 MA 144

Operando Phonon Studies of the Protonation Mechanism in Highly Active Hydrogen Evolution Reaction Pentlandite Catalysts — •Ioannis Zegkinoglou[1], Ali Zendegani[2], Ilya Sinev[1], Ulf-Peter Apfel[3], Tilmann Hickel[2], and Beatriz Roldan Cuenya[1] — [1]Department of Physics, Ruhr-University Bochum, Germany — [2]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [3]Inorganic Chemistry I, Ruhr-University Bochum, Germany

Synthetic pentlandite ($Fe_{4.5}Ni_{4.5}S_8$) is a promising electrocatalyst for hydrogen evolution, demonstrating high current densities, low overpotential, and remarkable stability in bulk form. The depletion of sulfur from the surface of this catalyst during the electrochemical reaction has been proposed to be beneficial for its catalytic performance. We have performed electrochemical operando studies of the vibrational dynamics of pentlandite under hydrogen evolution reaction conditions using ^{57}Fe nuclear resonant inelastic X-ray scattering [1]. Comparing the measured Fe partial vibrational density of states with DFT calculations, we have demonstrated that hydrogen atoms preferentially occupy substitutional positions replacing pre-existing sulfur vacancies. Once all vacancies are filled, the protonation proceeds interstitially, which slows down the reaction. Our results highlight the beneficial role of sulfur vacancies in the electrocatalytic performance of pentlandite and give insights into the hydrogen adsorption mechanism during the reaction. [1] I. Zegkinoglou et al., J. Am. Chem. Soc. 139, 14360 (2017).

CPP 54: Microswimmers (joint session BP/CPP/DY)

Time: Wednesday 15:00–17:30 Location: H 1028

Invited Talk CPP 54.1 Wed 15:00 H 1028

Emergent Dynamics of Active Particles — •Roland G. Winkler — Institute for Advanced Simulation, Forschungszemtrum Jülich, 52425 Jülich, Germany

The stationary-state structural and dynamical properties of microswimmers are governed by their shape and hydrodynamic interactions, but also the effective dimensionality of the system matters, i.e., three-dimensional bulk versus thin film. As a generic approach for microswimmers, we have developed a model for a spheroidal squirmer, with hydrodynamics implemented by the multiparticle collision dynamics approach [1,2]. We study the swimming behavior, cooperative motion, and motility-induced phase separation (MIPS) of such squirmers in a narrow slit. For two squirmers, surface hydrodynamic interactions strongly influences their cooperative motion [2]. Considering the phase behavior of many squirmers, hydrodynamic interactions suppress MIPS for spherical squirmers. In contrast, hydrodynamic interactions enhance MIPS for elongated squirmers. Moreover, the shape affects the rheological properties of squirmers in shear and Poiseuille flow.

[1] J. Elgeti, R. G. Winkler, G. Gompper, Rep. Prog. Phys. 78, 056601 (2015)

[2] M. Theers, E. Westphal, G. Gompper, R. G. Winkler, Soft Matter 12, 7372 (2016)

CPP 54.2 Wed 15:30 H 1028

Magnetic behavior and chemotaxis of magnetic bacteria — •Agnese Codutti[1], Damien Faivre[1], and Stefan Klumpp[2] — [1]Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14476 Potsdam, Germany — [2]Georg-August-Universität Göttingen Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Chemotaxis is the bacterial ability to bias their motility toward a preferred concentration of attractants or repellents. This chemotactic ability can be used by magnetic bacteria, coupling it to a passive alignment to external magnetic fields. Magnetic bacteria include the naturally-occurring magnetotactic bacteria, and lab-produced biohybrids, in which for example E. coli can be coupled to external magnetic beads. Therefore, a model to understand the coupling between magnetic fields, active swimming, and chemotaxis is needed to predict the behavior of these systems. We perform simulations based on an Active Brownian Particle model, modified to include active swimming, active changes of directions, chemotaxis, and passive alignment with external magnetic fields. The model allows us to reproduce the capillary experiments, and to throw some light on the possible aerotaxis models shown by magnetotactic bacteria. As main results, we show how run and tumble motion hinders the chemotactic/aerotactic abilities of the bacteria when coupled with magnetic fields, while run and reverse motility benefits from the magnetic field, leading to faster chemotaxis. We explore different magnetic behaviors of magnetotactic bacteria, where cells are either simply aligned by the external field or alternatively using it as proxy of oxygen gradient.

CPP 54.3 Wed 15:45 H 1028

The bacterial soliton in a nutrient field – re-examined — •Andrzej Palugniok[2], Maximilian Seyrich[1], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — [2]Worcester College, University of Oxford, Walton Street, OX1 2HB Oxford, United Kingdom

The gut bacterium *E. coli* with its run-and-tumble walk is a well-studied model swimmer in the active-matter field. One of the various interesting collective phenomena is a bacterial soliton or a traveling concentration pulse of bacteria [1]. It develops when bacteria start to consume a nutrient in an initially uniform field, in which they also perform chemotaxis.

To describe such a situation, we start from a Smoluchowski equation of a run-and-tumble particle in a chemotactic field. A Markovian tumble rate is derived from the usual linear response theory. We perform a multipole expansion to derive equations for the bacterial density and the local polar order decribed by the bacterial polarization. On times longer than the typical relaxation time for the polarization, one recovers the Keller-Segel equation. Solving it together with the diffusion equation for the nutrient, we are able to reproduce the bacterial soliton. Thereby, we demonstrate that one does not need a second, signalling chemical field as introduced in Ref. [1] nor a singular chemotactic drift term as demanded in Ref. [2].

[1] J. Saragosti et al., PNAS **108**, 39 (2011).
[2] E.F. Keller and L.A. Segel, J. Theor. Biol., **30**, 2 (1971).

CPP 54.4 Wed 16:00 H 1028

Dynamic Propulsion Force Measurements of Chlamydomonas Microalgae using Micropipette Force Sensors — •Thomas Josef Böddeker, Christian Titus Kreis, Quentin Magdelaine, and Oliver Bäumchen — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Faßberg 17, D-37077 Göttingen, Germany

Although the swimming dynamics of microbes, such as bacteria and microalgae, have received a lot of attention in recent years, methods for direct propulsion force measurements are still limited. We present a new approach utilizing micropipettes as force sensors to study the propulsion forces and wall interactions of the unicellular, biflagellated microswimmer *Chlamydomonas*. Fourier signal analysis of the micropipette deflection reveals a clear signature of the energy output of the microswimmer and provides a handle to measure the frequency and energy associated to the flagella beating. Continuous measurements in a liquid cell allow us to characterize the propulsion of individual cells and to probe the extent of steric and hydrodynamic interactions between beating flagella and solid interfaces. For controlled environmental conditions, we quantify the difference in propulsion energy and beating frequency between swimming in bulk and in close proximity to solid interfaces.

CPP 54.5 Wed 16:15 H 1028

Applying an Extended Kalman Filter to extract bacteria statistics — •Oliver Köhn — Universität des Saarlandes

Bacteria tend to swim in liquids in absence of food facilitated by creation of flagella. The trajectories are determined by slightly curved lines (running states) and randomly interrupted by short intervals with strong direction changes (tumbling state)[1]. This behavior seems to be efficient in finding food in unknown environments. We assume an intrinsic randomness in the running states as well in the appearance of the tumbling intervals.[1] Furthermore in real experiments the extracted positions are influenced by a detection noise. Estimating the stochastic trajectory properties requires the distinction between bacteria intrinsic randomness and the measurement noise. From the engineers it is known that the Kalmann filter algorithm provide this in an optimal way [2]. We adapted and implemented this filter for simulated as well as measured bacteria trajectories.

[1] Enhancing bacterial motility and search efficiency by genetic manipulation of flagellar number; Javad Najafi, M. Reza Shaebani, Thomas John, Florian Altegoer, Gert Bange & Christian Wagner; submitted to PNAS [2] Forecasting, structural time series models and the Kalman filter; Andrew C. Harvey; 1989; Cambridge University Press

CPP 54.6 Wed 16:30 H 1028

Phase diagram of a low Reynolds number swimmer near a wall — •Abdallah Daddi-Moussa-Ider[1], Maciej Lisicki[2,3], Christian Hoell[1], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, Düsseldorf 40225, Germany — [2]Department of Applied Mathematics and Theoretical Physics, Wilberforce Rd, Cambridge CB3 0WA, United Kingdom — [3]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

The hydrodynamic flow field generated by self-propelled active particles and swimming microorganisms is strongly altered by the presence of nearby boundaries in a viscous flow. Using a simple model swimmer composed of three-linked spheres, we show that the swimming trajectories near a non-slip wall reveal various interesting scenarios of motion depending on the initial orientation and the distance separating the swimmer from the wall. Accordingly, the swimmer can either be trapped by the wall, totally escape from the wall, or undergo an oscillatory gliding motion at a constant mean height above the wall. Using a far-field approximation, we find that the wall-induced correction at leading order has a quadrupolar flow structure where the translational and angular velocities of the swimmer decay as inverse third and fourth power with distance, respectively. The resulting equations of motion for the trajectories and the relevant order parameters fully characterize the transition between the phases and allow for an accurate description of the swimming behavior near a wall.

CPP 54.7 Wed 16:45 H 1028

Three-dimensional simulation of sperm in structured microfluidic channels — •Sebastian Rode, Jens Elgeti, and Gerhard Gompper — Theoretical Soft Matter and Biophysics, Institute of Complex Systems (ICS-2) , Forschungszentrum Jülich, 52425 Jülich, Germany

Sperm cells propel themselves by a periodic wave-like beating of their flagellum [1-3]. At low Reynolds numbers and in confinement, the directed motion of sperm and other microswimmers is strongly influenced by steric and hydrodynamic surface interactions [1]. We model sperm motility in our mesoscale hydrodynamics simulations by imposing a planar traveling bending wave along the flagellum [2]. For swimming in zigzag shaped microchannels, we find that the deflection angle of a sperm cell at sharp corners depends on the orientation of its beating plane. Our results are in good agreement with recent microfluidic experiments, and help to improve the understanding of sperm cell navigation under strong confinement. We show that the emergence of a nonplanar component of the flagellar beat with increasing wavelength drastically increases surface attraction.

[1] J. Elgeti et al., Rep. Prog. Phys. 78, 056601 (2015) [2] J. Elgeti et al., Biophys. J. 99, 1018 (2010) [3] G. Saggiorato et al., Nat. Commun. 8, 1415 (2017)

CPP 54.8 Wed 17:00 H 1028

Altering diffusion by interaction of microalgae with micronsized objects — •Francine Kolley[1,2], Patricia Dähmlow[2], Hajnalka Nadasi[2], Florian von Rüling[2], and Alexey Eremin[2] — [1]Technical University Dresden — [2]Otto-von-Guericke-University Magdeburg

The enhancement of passive particles, single silica spheres and their doublets, was studied in suspensions containing microswimmers Chlamydomonas reinhardtii. These green algae move with a flagellar motor, reaching typical velocities up to 150 μm/s. Stimulated by phototaxis, their motion is similar to humans doing breaststroke. The induced flow of the puller affects the translational as well as the rotational diffusion of the passive particles. The corresponding diffusion coefficients were obtained from the measurement of the mean square displacements of the passive particles for various concentrations of the algae. The Brownian Motion of the silica beads was observed in a quasi-2D system in flat cappilaries.To avoid cell immobilization by adsorption to the glass substrate the capillary surface was silanized. Additionally, a polymer was introduced to the suspension to optimize the diffusive behavior. In the range of small algae concentrations, the diffusion coefficients exhibited a linear dependence on the cell density of Chlamydomonas reinhardtii.

CPP 54.9 Wed 17:15 H 1028

Dynamics of chemotactic and chemokinetic bacterial populations — •Theresa Jakuszeit[1], James Lindsey-Jones[1], François J. Peaudecerf[2], and Ottavio A. Croze[1] — [1]Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom — [2]Institute of Environmental Engineering, ETH Zürich, Stefano-Franscini-Platz 5, 8093 Zürich, Switzerland

Several motile bacteria are able to sense chemical gradients much larger than their own size, and perform a random walk biased up attractant gradients ('chemotaxis') by varying their reorientation rate. In addition to this well-known chemotactic behaviour, several soil and marine bacterial species are known to modify their swimming speed according to the local concentration of chemoattractant ('chemokinesis'). Therefore, a chemical field of attractant induces a spatially varying swimming speed, which results in a drift towards lower attractant concentrations – contrary to the drift created by chemotaxis.

Here, to explore the biological benefits of chemokinesis and investigate its impact on the chemotactic response, we extend a Keller-Segel type model to include a dependence of the swimming speed on the attractant concentration. Even though chemokinesis on its own results in a dispersion of the population away from high attractant concentrations, it can not only enhance the chemotactic response but also modify it qualitatively. We apply the model to predict the dynamics of bacteria capable of chemokinesis and chemotaxis in experimentally inspired chemoattractant fields, such as those generated in capillary migration assays and around environmental nutrient sources.

CPP 55: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials V (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Wednesday 15:00–17:45 Location: HL 001

Invited Talk CPP 55.1 Wed 15:00 HL 001

Computational Approach to the Electronic Structure of Strongly Correlated Materials: Towards Theoretical Spectroscopy and Theory Assisted Material Design — •Gabriel Kotliar — Serin Physics Laboratory Rutgers University — Brookhaven National Laboratories

We will introduce a project, to build algorithms and a suite of open source codes, to compute the electronic structure of correlated materials. It involves different methods, to provide different compromises between speed and accuracy, and to treat different types of correlation (static and dynamic). The suite includes methods ranging from vertex corrected GW, rotationally invariant slave bosons and LDA+DMFT, and we will illustrate some of these methods (and their failures) in d and f electron systems.

CPP 55.2 Wed 15:30 HL 001

Spectral properties of Sr2IrO4 from first principles — •Cyril Martins[1], Benjamin Lenz[2], and Silke Biermann[2,3] — [1]Laboratoire de Chimie et Physique Quantiques, UMR 5626, Université Paul Sabatier, 118 route de Narbonne, 31400 Toulouse, France — [2]Centre de Physique Théorique, Ecole Polytechnique, CNRS UMR 7644, Université Paris-Saclay, 91128 Palaiseau, France — [3]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

The spin-orbit system Sr2IrO4 has raised tremendous interest recently, due to intriguing similarities to the high-Tc superconducting copper oxides.

We study the evolution of the electronic structure of Sr2IrO4 using a combination of ab-initio density functional theory and many-body techniques. The effects of spin-orbit coupling, distortions of the oxygen octahedra and Hubbard interactions are included on a first-principles level. We calculate the momentum-resolved spectral function and compare to recent photoemission data, finding good agreement with experiment.

CPP 55.3 Wed 15:45 HL 001

Role of non-local correlations in doped Sr_2IrO_4 — •Benjamin Lenz[1], Cyril Martins[2], and Silke Biermann[1,3] — [1]Centre de Physique Théorique, Ecole Polytechnique, CNRS UMR 7644, Université Paris-Saclay, 91128 Palaiseau, France — [2]Laboratoire de Chimie et Physique Quantiques, UMR 5626, Université Paul Sabatier, 118 route de Narbonne, 31400 Toulouse, France — [3]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

When doping the spin-orbit system Sr_2IrO_4 recent photoemission experiments found pseudogap behavior at low temperatures, which raises the question of its relation to the pseudogap found in high-Tc superconducting copper oxides.

Here, we study the evolution of the electronic structure of Sr_2IrO_4 upon electron- and hole-doping by combining ab-initio density functional theory and two quantum cluster techniques. Our treatment includes the effects of spin-orbit coupling, distortions of the oxygen octahedra and Hubbard interactions on a first-principles level. We show that short-range antiferromagnetic fluctuations are crucial to account for the electronic properties of the material even in the high-temperature paramagnetic phase. Furthermore, pseudogap features in the momentum-resolved spectral function of the emerging exotic metallic state are analyzed and found to be in good agreement with experiment.

CPP 55.4 Wed 16:00 HL 001

Describing the coupled structural and metal-insulator transition in rare-earth nickelates with DFT+DMFT — •Alexander Hampel and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

Perovskite rare-earth nickelates, $R\mathrm{NiO}_3$, display a rich phase diagram, where all compounds with R from Pr to Lu undergo a metal-insulator transition (MIT) that is accompanied by a structural distortion. This distortion breaks the symmetry between formerly equivalent Ni sites and is related to a charge disproportionation driven by correlation effects, resulting in an insulating state. Here, we employ density functional theory together with dynamical mean field theory (DFT+DMFT) to explore the interplay between lattice distortions and electronic correlation effects in these compounds. By utilizing a symmetry-based distortion mode analysis, we are able to isolate the specific lattice distortion occurring at the phase transition. Calculating total energies within DFT+DMFT then allows us to relax the structures with respect to this distortion. We find, that the resulting distortion amplitudes and its variation across the series are in good agreement with experimental results. Our work highlights the capabilities of the DFT+DMFT method to describe complex materials with coupled electronic and structural degrees of freedom.

CPP 55.5 Wed 16:15 HL 001

Magnetocrystalline anisotropy of FePt: LDA+DMFT study — •saleem Ayaz Khan[1], Junqing Xu[2], johan Schott[3], Ondřej Šipr[1], and Jan Minár[1] — [1]University of West Bohemia, Pilsen, Czech Republic — [2]LMU Munich, Germany — [3]Uppsala University, Sweden

In our recent work (Phys. Rev B, 94, 144436, 2016) we employed ab initio methods (FLAPW and KKR) to get a reliable value for the magnetocrystalline anisotropy (MCA) energy of FePt. The theoretical MCA energy of FePt (3.0 meV) is significantly larger than the experimental value (1.3 meV), implying that the LDA cannot properly describe the MCA of FePt. Considering that the MCA essentially arises from spin orbit coupling it appears that to obtain reasonable agreement with experiments, it is necessary to include orbital correlations. To account realistically for both the electronic and geometric structure of materials, we use a combined density functional and dynamical mean field theory, LDA+DMFT. Our computation is based on the fluctuation exchange approximation and an analytic continuation method for the self-energy. Our results show that dynamical correlation effects are important for a correct treatment of the 3d-5d hybridization in FePt, which in turn plays a significant role for the magnetocrystalline anisotropy

CPP 55.6 Wed 16:30 HL 001

Diagnostics for plasmon satellites and Hubbard bands in transition metal oxides — •Steffen Backes[1], Hong Jiang[2], and Silke Biermann[1] — [1]Centre de Physique Théorique, École Polytechnique, 91128 Palaiseau, France — [2]College of Chemistry and Molecular Engineering, Peking University, China

The generally accepted picture of $SrVO_3$ is that of a correlated electron metal where a renormalized quasi-particle peak at the Fermi level coexists with upper and lower Hubbard bands, separated by Coulomb interaction U. Recently, this picture has become blurred with the rise in interest in additional plasmonic satellites. Distinguishing plasmonic features from Hubbard bands is a non-trivial question. In this talk we employ combined many-body perturbation theory and dynamical mean field theory ("GW+DMFT") to discuss the processes that give rise to these different satellites and show how to identify their origin in realistic materials. We present an application of this scheme to different transition metal oxides, which we find to exhibit both Hubbard and plasmonic satellites at similar energetic positions.

CPP 55.7 Wed 16:45 HL 001

Phase transitions of the 2D Hubbard-Holstein model — •Teresa E. Reinhard[1], Uliana Mordovina[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

In the 2d Hubbard-Holstein model at zero temperature, a quantum phase transition between Mott and Peierls insulator can be observed. Whether a metallic phase emerges in between remains an open question [1,2]. As the emergence of the Mott phase is a many body effect, a description beyond the mean field level is crucial. At the same time, a method that can cope with two dimensions is needed.

To address this open question, we have extended Density Matrix Embedding Theory (DMET) from the purely electronic case [3,4] to coupled fermion-boson systems. DMET is an embedding theory which benefits from the exponentially decaying correlation in most quantum systems thus allowing a description beyond mean field at low cost.

We show the phase diagram of the 2d Hubbard-Holstein model at zero temperature obtained for different cluster sizes. [1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012) [2] S. Wouters, C. A. Jiménez-Hoyos, G. K.-L. Chan, arXiv:1605.05547 (2016) [3] R. T. Clay and R. P. Hardikar, Phys. Rev. Lett 95, 096401 (2005) [4] J. Bauer, EPL 90 27002 (2010)

CPP 55.8 Wed 17:00 HL 001

A quantum embedding theory combining many-body perturbation theory with configuration interaction — •Marc Dvorak and Patrick Rinke — Department of Applied Physics, Aalto University School of Science, 00076-Aalto, Finland

We present a new quantum embedding theory called dynamical configuration interaction (DCI). It captures non-local and static correlation in an orbital active space with configuration interaction (CI) and high-energy, dynamic correlation in the complementary bath space with many-body perturbation theory (MBPT). The formulation is general, but we focus on molecular systems with an *ab-initio* Hamiltonian. The conceptual key to our approach is to replace the exact electronic Hamiltonian in the bath space with one of excitations defined over the correlated ground state. This transformation is naturally suited to the language and methodology of many-body Green's functions. Correlation in the bath is therefore described at the quasiparticle level with Green's functions instead of with the many-body wave function. Our approach avoids computational and conceptual difficulties associated with Green's function embedding and improves upon wave function methods by including dynamical correlation from the bath space. A major advantage to DCI is that it naturally treats ground and excited states on equal quantum mechanical levels. For ground state properties, we present dimer dissociation curves for H_2 and N_2 in excellent agreement with exact results. Excited states of N_2 give excellent agreement with experiment, and we demonstrate the scalability of our method by computing excited states of a free-base porphyrin molecule.

CPP 55.9 Wed 17:15 HL 001

Real-Structure Effects and Correlation in Layered Sodium Cobaltates — Sophie Chauvin[1,2], Silke Biermann[1], Lucia Reining[2], and •Claudia Rödl[3] — [1]Centre de Physique Théorique, École polytechnique, CNRS, Université Paris-Saclay, 91128 Palaiseau, France — [2]Laboratoire des Solides Irradiés, École polytechnique, CNRS, CEA, Université Paris-Saclay, 91128 Palaiseau, France — [3]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Na-doped layered cobaltates Na_xCoO_2 feature a rich phase diagram with a plethora of physical phenomena ranging from metal-insulator transitions over magnetism to charge ordering. These instabilities of the electronic structure are mostly attributed to correlation effects within the quasi-2D CoO_2 layers. Here, we focus on $Na_{2/3}CoO_2$, a doping for which the system is metallic and exhibits an experimentally established charge disproportionation on the Co atoms.

We study the electronic properties of the CoO_2 layers and investigate the impact of the intercalated Na atoms on the electronic structure in the ordered layered superstructure. The problem is tackled from an *ab-initio* point of view using density-functional theory (DFT) and many-body perturbation theory (MBPT). Moreover, we study the static charge-density response of the material to understand instabilities in the system. Our approach complements recent model calculations from extended dynamical mean-field theory (EDMFT). The calculated results are compared to experimental spectroscopic data.

CPP 55.10 Wed 17:30 HL 001

Slave rotor approach to impurity models with correlated dp orbitals — •Jakob Steinbauer and Silke Biermann — École Polytechnique, Palaiseau, France

We propose a slave rotor method for the solution of many-orbital quantum impurity problems, which maps the original problem onto one with reduced degeneracy. This is particularly useful for the dynamical mean field theory treatment of transition metal oxides where the interactions between ligand states with d-electrons are all too often simply neglected. We derive a general formalism relying on an optimized effective model obtained from the variational principle of Feynman and Peierls and test the method in the atomic limit.

CPP 56: Materials for Energy Storage II (joint session KFM/CPP)

Organizer: Martin Diestelhorst - Martin-Luther-Universität Halle-Wittenberg - Halle

Time: Wednesday 15:00–17:50 Location: EMH 025

Invited Talk CPP 56.1 Wed 15:00 EMH 025

Electrical double layer capacitors, Insights from fundamental research and their impact on storage devices — •Gudrun Reichenauer — Bavarian Center for Applied Energy Research, 97074 Wuerzburg, Germany

Electrical double layer capacitors (EDLC) are important components in the toolbox of currently available electrical storage devices, serving in particular applications that require reliability and high power density, such as e.g. emergency doors in airplanes, or high cycling stability at low to medium energy density, such as electrically driven buses for public transportation. Typically, optimization of EDLCs is performed by empirical tests of different active materials, binders and conductive additives. However, only limited systematic studies are available to address questions, such as

What are the optimized structures in terms of pore sizes and porosity of the active component?

How do the micropore (pores < 2 nm) characteristics affect the storage in the presence of organic, aqueous and polymer electrolytes?

What is the impact of the device layout vs. the properties of the electrode itself on the performance (energy and power density) of an EDLC?

The talk will address some of these questions using model carbon materials that allow systematic variation of key parameters and also show how new in-situ/in-operando techniques can further support a more targeted development of EDLC storage devices for different types of applications.

CPP 56.2 Wed 15:30 EMH 025

Pyrolytic graphite electrodes intercalated by $AlCl_4$ anions probed by X-ray tomography and small angle X-ray scattering — •Giorgia Greco[1], Giuseppe Elia[2], Dragomir Tachev[3], Armin Hoell[1], Robert Hahn[4], and Simone Raoux[1,5] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany — [2]. Technische Universität Berlin, Research Center of Microperipheric Technologies, Gustav-Meyer-Allee 25, 13355 Berlin, Germany — [3]Institute of Physical Chemistry, Bulgaria Academy of Science, Acsd. G. Bonchev Str. Bl.11, 1113 Sofia, Bulgaria — [4]. Fraunhofer-Institut für Zuverlässigkeit und Mikrointegration , Gustav-Meyer-Allee 25, 13355 Berlin, Germany — [5]. Department of Physics, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Due to the cost and limited resources of lithium, the use of Li-ion batteries for large scale applications is nowadays under discussion. Aluminum based secondary batteries could be a viable alternative to the present Li-ion technology because of their high volumetric capacity. Additionally, the low cost aluminum makes these devices appealing for large-scale electrical energy storage. We report the structural characterization by a combination of x-ray tomography and SAXS (Small Angle X-ray Scattering) related to electrochemical performances of aluminum tetrachloride electrolyte in an aluminum/graphite battery. The aim of this work is to characterize the micro- and nano-structure of highly ordered graphite during the electrochemically induced reaction mechanism of $AlCl_4$ intercalation.

CPP 56.3 Wed 15:50 EMH 025

Structural and microstructural evolution during oxygen intercalation in $Pr_2NiO_{4.25}$ single crystal investigated by in-situ synchrotron diffraction — •Avishek Maity[1,2], Rajesh Dutta[3], Monica Ceretti[3], Dmitry Chernyshov[4], and Werner Paulus[3] — [1]Institut für Physikalische Chemie, Georg-August Universität Göttingen, 37077 Göttingen, Germany — [2]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), 85748 Garching, Germany — [3]Institut Charles Gerhardt, Université de Montpellier, 34095 Montpellier, France — [4]The European Synchrotron-ESRF, 38000 Grenoble, France

Pr_2NiO_{4+x} is a promising oxygen membrane material having excellent ionic conductivity at moderate T. Oxygen diffusion occurs through interstitial sites via phonon assisted diffusion mechanism. We found $Pr_2NiO_{4.25}$ to be structurally extremely complex, showing large oxygen (interstitial) and charge (Ni^{2+}/Ni^{3+}) ordered domains, and forming giant unit cells up to 6000000 Å^3. In order to explore the oxygen diffusion from structural and microstructural aspect as a function of oxygen stoichiometry ($0<x<0.25$), we investigated in-situ electrochemical (EC) oxygen intercalation on a 50 micron highly twinned single crystal mounted in a specially designed EC cell using synchrotron diffraction at BM01A@ESRF. We have followed phase transitions (ortho → tetra → ortho) and evolution of domain structure with a very special focus on the presence or absence of grain boundaries. This insitu study allowed during an EC reaction to explore whole reciprocal space i.e. microstructure, twin domains including diffuse scattering.

CPP 56.4 Wed 16:10 EMH 025

A green magnetic cooling device built using upcycled NdFeB magnets — •Dimitri Benke[1], Jonas Wortmann[1], Marc Pabst[1], Tino Gottschall[2], Iliya Radulov[1], Konstantin Skokov[1], Oliver Gutfleisch[1], Davide Prosperi[3], Peter Afiuny[3], and Miha Zakotnik[3] — [1]TU Darmstadt, Darmstadt, Deutschland — [2]Helmholtz-Zentrum Dresden-Rossendorf, Rossendorf, Deutschland — [3]Urban Mining Company, Austin, USA

Magnetocaloric devices hold the potential to satisfy the rising demand for cooling in the future. One remaining challenge is to reduce the high ecological footprint of the permanent magnets driving the magnetic cooling cycle. Existing devices use neodymium-iron-boron (NdFeB)-type permanent magnets, which account for more than 50% of the ecological footprint of the appliance. To overcome this hurdle, TU Darmstadt and Urban Mining Company have built the first working magnetocaloric device that uses recycled NdFeB as a magnetic field source. Coupling this with optimisation of the magnets and their geometry, it is possible to further reduce the ecological footprint. Together, these two approaches help to position magnetic cooling as a realistic and sustainable cooling technology.

20 min. break

CPP 56.5 Wed 16:50 EMH 025

Electromagnetic Functionalization of Wide Band Gap Dielectric Oxides by Interstitial Doping — •Dae-Sung Park[1,3], Haiyuan Wang[2], Diana Rata[3], Akash Bhatnagar[1,3], Igor Maznichenko[3], Sergey Ostanin[3], and Kathrin Dörr[3] — [1]Zentrum für Innovationskompetenz SiLi-nano, Halle, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [3]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

In solid-state oxides, methods such as chemical doping/alloying, mechanical strain, defect engineering, and integration of distinct materials, have been conventionally used to modify a wide range of physical and chemical properties. Here, we demonstrate an extraordinary interstitial doping effect centred around a light element (boron) cation. The host matrix is a novel composite system synthesised from discrete bulk LaAlO3:LaBO3 compounds. Our results show a spontaneous ordering of the interstitial boron cations within the host LaAlO3 lattices, and subsequent effective spin-polarized charge injection into the neighbouring cations. These ordered interstitials lead to a series of remarkable functional properties, namely, cation-dominated electrical switching and ferromagnetism. Therefore, interstitial boron doping serves to transform a wide band gap and non-magnetic dielectric bulk oxide into a high-temperature ferromagnetic ionic-electronic conductor. This interstitial doping effect is proposed to be a general route for tailoring new multifunctional properties in bulk oxides for smart materials applications such as non-volatile information and spintronic devices.

CPP 56.6 Wed 17:10 EMH 025

The impact of different Si surface terminations in the (001) n-Si/NiOx heterojunction on the oxygen evolution reaction (OER) by XPS and electrochemical methods — •Sven Tengeler, Mathias Fingerle, Wolfram Calvet, Céline Steinert, Bernhard Kaiser, Thomas Mayer, and Wolfram Jaegermann — Technische Universität Darmstadt

The interaction between (001) n-Si and NiOx was investigated with regard to the oxygen evolution reaction (OER), applicable either for water splitting or CO2 reduction. Thin layers of NiOx were deposited step by step by reactive sputter deposition and analyzed in-situ after each step using X-ray photoelectron spectroscopy (XPS) for Si with different surface preparations: H-termination, thermally grown oxide (2 Å) and native oxide (4 Å). Upon contact formation the initial flat band like situation in the Si substrates changed to a 0.35-0.4 eV upward band bending for all three heterojunctions, hole extraction barriers are low.

The observed similarities in the heterojunctions should result in the same similarities for the OER performance. However, cyclic voltammetry measurements reveal a shift of more than 0,2 V in dependence of the surface treatment. Using chopped light measurements, this underperformance could be attributed to a higher density of defect states at the Si surface. Apparently a 4 Å SiO2 layer is sufficient protection to prevent the formation of defect states during NiOx deposition, thinner protective layers or none at all result in increased defect states, while thicker layers perform poorly due to their high ohmic resistance.

CPP 56.7 Wed 17:30 EMH 025

Interaction of water with wet-chemically etched p-GaInP2(100) surface — Andreas Hajduk[1], •Mikhail Lebedev[2], Bernhard Kaiser[1], and Wolfram Jaegermann[1] — [1]TU Darmstadt, AG Oberflächenforschung, Otto-Berndt-Straße 3, 64287 Darmstadt — [2]Ioffe Institute, Politekhnicheskaya 26, St. Petersburg, 194021 Russia

Photoelectrochemical water splitting offers the possibility to convert solar energy directly into a chemical fuel and therefore is a promising candidate for a sustainable energy solution in the future. GaInP2 with a direct bandgap of 1.8-1.9 eV shows so far the highest reported solar-to-hydrogen conversion efficiencies. Nevertheless, the fast photocorrosion of III-V semiconductors in aqueous solution presents a major obstacle for their use as efficient and stable photoelectrodes. Interaction of water with chemically etched p-GaInP2(100) surface covered with a submonolayer of residual oxides is studied by synchrotron photoemission spectroscopy to gain insight into the solid/solvent interaction at the semiconductor/electrolyte interface. Photoemission spectra obtained after emersion of the semiconductor from liquid water at room temperature and adsorption of H2O molecules at liquid-nitrogen temperature are compared to understand the chemistry of the GaInP2(100)/H2O interface. Valence band spectra indicate dissociative adsorption of water molecules both after emersion and after adsorption experiments. Surface-sensitive core level spectra reveal the interaction of H2O molecules with surface phosphorous and gallium atoms.

CPP 57: Active Matter (joint session DY/CPP/BP)

Time: Wednesday 15:30–18:45 Location: BH-N 243

CPP 57.1 Wed 15:30 BH-N 243

Three-body correlations and conditional forces in suspensions of active hard disks — •Andreas Härtel[1], David Richard[2], and Thomas Speck[2] — [1]University of Freiburg, Freiburg, Germany — [2]Johannes Gutenberg-University Mainz, Mainz, Germany

Self-propelled Brownian particles show rich out-of-equilibrium physics, but while decades of studying the structure of liquids have build up a deep understanding of passive systems, not much is known about correlations in active suspensions. For this reason, we derive an approximate analytic theory for three-body correlations and forces in systems of active Brownian disks starting from the many-body Smoluchowski equation. Via this theory we discuss properties of conditional three-body forces, an effective swimming speed, and pair distributions. We further test and validate our theory using particle-resolved computer simulations. They allow us to discuss the modeling of active Brownian swimmers with nearly hard interaction potentials. We finally define appropriate parameters to describe active systems and discuss them as a basis for further studies of correlations in active suspensions and for an emerging liquid state-theory.

CPP 57.2 Wed 15:45 BH-N 243

Giant Kovacs-Like Memory Effect for Active Particles — •Rüdiger Kürsten[1], Vladimir Sushkov[2], and Thomas Ihle[1] — [1]Universität Greifswald — [2]Hochschule für angewandte Wissenschaften München

Dynamical properties of self-propelled particles obeying a bounded confidence rule [1] are investigated by means of kinetic theory and agent-based simulations. While memory effects are observed in disordered systems, we show that they also occur in active matter systems [2]. In particular, we find that the system exhibits a giant Kovacs-like memory effect that is much larger than predicted by a generic linear theory. Based on a separation of time scales we develop a nonlinear theory to explain this effect. We apply this theory to driven granular gases and propose further applications to spin glasses.

[1] Phys. Rev. E 90, 063315 (2014)

[2] Phys. Rev. Lett. 119, 188001 (2017)

CPP 57.3 Wed 16:00 BH-N 243

Active Brownian Particles in Crowded Media — •Jonathan Ónody[1], Alexander Liluashvili[1], and Thomas Voigtmann[1,2] — [1]Deutsches Zentrum für Luft- und Raumfahrt e.V, Köln, Deutschland — [2]Fachgruppe Physik, Heinrich-Heine Universität, Düsseldorf, Deutschland

We investigate the dynamics of model microswimmers (active Brownian particles) evolving at high densities and in the presence of crowding, i.e., in model porous media, making use of the mode-coupling theory of the glass transition (MCT). The microswimmers are modeled by hard disks in two dimensions undergoing both, translational and rotational diffusion. In addition they posses a constant self-propulsion velocity in their direction of orientation. MCT predicts an idealized active-glass transition, and we discuss the features of the slow dynamics emerging close to that transition. The porous background is treated as a frozen disordered density field. We discuss the structure of the resulting theory, distinguishing between connected and disconnected parts of the correlation functions.

1. Liluashvili, A., Ónody, J., and Voigtmann, Th., Mode Coupling Theory for Active Brownian Particles, Phys. Rev. E in press, arXiv:1707.07373 (2017).
2. Krakoviack, V., Mode-coupling theory for the slow collective dynamics of fluids adsorbed in disordered porous media, Phys. Rev. E 75, 031503 (2007).
3. Götze, W., Complex Dynamics of Glass-Forming Liquids - A Mode-Coupling Theory

CPP 57.4 Wed 16:15 BH-N 243

Cans and cannots of heat engines with nonequilibrium baths — •stefano steffenoni[1], viktor holubec[2], gianmaria falasco[3], and klaus kroy[2] — [1]Max Planck for the Mathematics in the Science, leipzig — [2]Institute for Theoretic Physics, Leipzig — [3]University of Luxembourg, Luxembourg

We investigate a heat engine based on a Brownian colloid, confined in a parabolic potential and coupled to an active particles bath. The energetics of the cycle is governed by the variance of the colloid distribution. With a suitable definition of a time-dependent effective temperature, it obeys the same dynamical equation as a passive colloid coupled to a conventional thermal bath. Performance of the active heat engine including maximum efficiency, efficiency at maximum power and maximum efficiency at a fixed power can thus all be understood from ordinary thermodynamics, using the appropriate effective temperature. On this basis, we provide a thorough analysis of recent experiments (Krishnamurty et al. Nat. Phys. 2016) that lead to the spectacular claim that thermodynamic cycles coupled to active baths can surpass the ultimate efficiency of an equilibrium Stirling cycle.

CPP 57.5 Wed 16:30 BH-N 243

Dynamics of self-propelled granular particles on a vibrated plate — •Tina Hanselka and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg

Screws sliding on a periodically vibrating plate can be used as a very simple model system to examine the motion of self-propelled particles in 2D. We analyze the active Brownian motion a single screw performs, then we explore the self-organization of large groups of particles, focusing on mixtures between active and passive materials, realized by screw nuts of comparable weights.

15 min. break

CPP 57.6 Wed 17:00 BH-N 243

Diffusive dynamics of complex colloidal particles in active suspensions of microswimmers — •Florian von Rüling, Francine Kolley, Patricia Dähmlow, Hajnalka Nadasi, and Alexey Eremin — Otto von Guericke University Magdeburg

We report experimental studies on the active motion of puller-type microswimmers Chlamydomonas reinhardtii (C.R.) and the entrainment and the diffusion of complex passive particles in thin capillaries. C.R., self-propelled unicellular alga, swims in the regime of low Reynolds number due to its flagellar motion breaking time-reversal symmetry. Having an eyespot, the alga shows phototactic behaviour. Employing a particle tracking algorithm and polarising microscopy, we explore the enhancement of the diffusion of the sphere- and rod-shaped particles by swimming algae. Furthermore, we demonstrate the effect of the microswimmer-induced flow on the director field of nematic droplets dispersed in the active colloid.

CPP 57.7 Wed 17:15 BH-N 243

Self-spinning particles phase separate and move collectively — •Christian Scholz[2,1], Michael Engel[1], and Thorsten Pöschel[1] — [1]Institute for Multiscale Simulation, FAU Erlangen, Germany — [2]Institut für Theoretische Physik 2, HHU Düsseldorf, Germany

We create 3d-printed minimalistic robots that perform self-spinning motion. Binary mixtures of clockwise and counter-clockwise spinning particles phase separate and exhibit collective ballistic motion along the interfaces. We compare our experimental system to Langevin simulations to demonstrate that our macroscopic system is a form of active soft matter. Simulations also allow us to demonstrate that confinement in the system, on long time scales, favors symmetric demixing patterns.

CPP 57.8 Wed 17:30 BH-N 243

Entropy production of active particles and for particles in active baths — •Patrick Pietzonka[1,2] and Udo Seifert[1] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, Germany — [2]Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK

Entropy production of an active particle in an external potential is identified through a thermodynamically consistent minimal lattice model that includes the chemical reaction providing the propulsion and ordinary translational noise. In the continuum limit, a unique expression follows, comprising a direct contribution from the active process and an indirect contribution from ordinary diffusive motion. From the corresponding Langevin equation, this physical entropy production cannot be inferred through the conventional, yet here ambiguous, comparison of forward and time-reversed trajectories. Generalizations to several interacting active particles and passive particles in a bath of active ones are presented explicitly, further ones are briefly indicated. [1] P. Pietzonka and U. Seifert, J. Phys. A: Math. Theor. **51**, 01LT01 (2018)

CPP 57.9 Wed 17:45 BH-N 243

Binary Mixtures of Active and Passive Particles — •Francesco Alaimo[1,2] and Axel Voigt[1,2,3] — [1]Institut für Wissenschaftliches Rechnen, TU Dresden, Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany — [3]Center for Systems Biology Dresden (CSBD), Dresden, Germany

We use a modification of the Binary Phase Field Crystal model to introduce a continuous approach for binary mixtures of passive and active particles.

This continuous model is used to numerically study different effects that arise in binary mixtures. First, we see how activity promotes crystallization and cluster formation in a passive system, a phenomenon that has been observed experimentally. By varying the relative densities we can observe how passive obstacles influence the dynamics of active particles. Finally, we show how, under specific conditions, a crowded environment can lead to a partial trapping of active particles.

CPP 57.10 Wed 18:00 BH-N 243

Phase diagram, capillary waves, and interfacial stiffness of active-passive polymer mixtures — •Jan Smrek, Kostas Daoulas, and Kurt Kremer — Max Planck Institute for Polymer Research, Mainz, Germany

The active-passive polymer mixtures serve as a model for phase separation of transcriptionally active and inactive DNA strands in nuclei of living cells. Is it possible to distinguish the equilibrium phase separation, driven by chemical differences, from the non-equilibrium one? Here, we study the interfacial properties of the phase separated steady states of the scalar active-passive polymer mixtures. We construct phase diagrams and extract the analogue of the equilibrium critical exponent β governing the density difference. Looking at the interface fluctuations, we find they follow the equilibrium capillary waves spectrum. This allows us to establish a mechanistic definition of the non-equilibrium interfacial stiffness and its dependence on the activity asymmetry. We show how the interfacial width depends on the activity ratio and comment on the finite size effects. Our results show the non-equilibrium steady state behaves in many respects as an equilibrium polymer mixture with LCST.

CPP 57.11 Wed 18:15 BH-N 243

High-motility light-driven AgCl Janus microswimmers interacting with passive beads — •xu wang[1], Larysa Baraban[2], Annie T. Phuong Nguyen[2], Jin Ge[1], Vyacheslav Misko[3], Gianaurelio Cuniberti[2], Jürgen Fassbender[1], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, 01328 Dresden, Germany — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — [3]Department Fysica, Universiteit Antwerpen, B-2020 Antwerpen, Belgium

Visible light driven nano/micro swimmers are promising candidates for potential biomedical and environmental applications, which have been highlighted in the study of manmade nanao/micro swimmers stimulated by versatile light sources.1-5 To increase the motile speed, Janus polystyrene (PS)/AgCl microswimmers have been developed, which are capable to be actuated and tuned by blue light and achieve a high moving speed with 7 μm/s in pure water. To understand the interaction mechanism between artificial microswimmers and the surrounding environment, with the stimuli of blue light, prepared clusters composed of different numbers of Janus PS/AgCl particles and PS beads are used as active and passive motile objectives for sub-systematic models. The dynamics of a single Janus particle, single Janus particles assemblies, collective behaviours have been investigated and demonstrated both with experimental and simulated results.

CPP 57.12 Wed 18:30 BH-N 243

High-motility visible light-driven AgCl Janus microswimmers interacting with passive beads — •Xu Wang[1], Larysa Baraban[2], Annie T. Phuong Nguyen[2], Jin Ge[1], Vyacheslav Misko[3], Gianaurelio Cuniberti[2], Jürgen Fassbender[1], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, 01328 Dresden, Germany — [2]Dresden University of Technology, 01062 Dresden, Germany — [3]Universiteit Antwerpen, B-2020 Antwerpen, Belgium

Visible light driven nano/micro swimmers are promising candidates for different applications. However, the previous obtained mean squared displacement (MSD) values are low (up to 200 squared micrometers (10 s)) even under the favorable UV light illumination.[1,2] This is a severe drawback for the applications where the efficient transport of microswimmers is demanded.

We demonstrate AgCl based spherical Janus microswimmers reveal an efficient propulsion under blue (visible) light (λ=450-490 nm)illumination. The proper design of a AgCl based microswimmer can boost the MSD to 3000 squared micrometers (10 s) in pure H2O. We investigate the motion of individual Janus particles as well as their small (3-particles) and large (many particles) clusters. With experimental results and numerical simulations (by Langevin equations), we provide an insight into the collective behavior of the Janus microswimmers surrounded by polystyrene (PS) beads.

1. Angew.Chem.Int.Ed. 2009,48,3308. 2. ChemNanoMat 2017,3,65.

CPP 58: Organic Thin Films, Organic-Inorganic Interfaces: Session I (joint session DS/CPP)

Time: Wednesday 16:00–18:15 Location: H 0111

Invited Talk CPP 58.1 Wed 16:00 H 0111

Prospects of Engineering Chemistry and Electronic Character of Interfaces in Multifunctional (Bio)Organic-Inorganic Hybrids — •Maria Losurdo — Institute of Nanotechnology, CNR-NANOTEC, Bari, Italy

New opportunities for energy harvesting, plasmonics, active photonics, biomimetic catalysis, biosensing, immunosensing and cellular recognition are offered by novel hybrid heterojunctions combining, semiconductors, plasmonic metal nanostructures and (bio)-organic systems.

In order to design these (bio)-organic/inorganic platforms, the establishment of reliable and reproducible protocols for their functionalization is still needed, which require better understanding of the surface and interfacial electronic phenomena.

This contribution presents strategies for tailoring the chemistry and electronic character of interfaces in hybrids spanning from planar surfaces (semiconductors Si, III-Vs, TCOs, SiC) to nanosystems (plasmonic Au, Ga, Al) designed to enable applications in photovoltaics (hole transport organic layers and semiconducting new polymers), biomimetic catalysis (porphirins) and bio- immuno-sensing (proteins, DNA, cells).

The emphasis will be on functionalization methods, including plasma treatments of surfaces and interfaces, resulting assembly and nanostructures and how the interface chemistry determines the charge transfer enabling the specific functionality.

Future directions towards the rational design of those hybrids will be suggested.

15 min. break.

CPP 58.2 Wed 16:45 H 0111

Synthesis and combined experimental and theoretical characterization of dihydro-tetraaza-acenes — •Bernd Kollmann[1], Zhongrui Chen[2], Daniel Lüftner[1], Olivier Siri[2], and Peter Puschnig[1] — [1]Institute of Physics, University of Graz, NAWI-Graz, Universitätsplatz 5. 8010 Graz, Austria — [2]Aix Marseille Universite, CNRS, CINaM UMR 7325, 13288 Marseille, France

We present a combined experimental and theoretical study of electronic and optical properties of dihydro-tetraaza-acenes (DHTAn). Using a solvent-free condensation, we are able to synthesize DHTA5, DHTA6 and DHTA7 molecules. We investigate their gas-phase electronic structures of by means ab-initio density functional calculations employing an optimally-tuned range-separated hybrid functional. By comparing with the parent linear oligoacenes (nA) and based on computed ionization potentials and electron affinities, we predict DHTAn molecules to be more stable than acenes of the same length, where we expect DHTAn molecules to be persistent at least up to n = 7 rings. We further exploit the analogy with nA by analyzing the entire intramolecular π-band structure of the DHTAn molecules. This clearly reveals that the additional two electrons donated by the dihydropyrazine group are delocalized over the entire molecule and contribute to its π-electron system. As a consequence, the symmetry of the frontier orbitals of DHTAn differs from that of the parent nA molecule. This is also illustrated by the UV-vis absorption spectra which have been measured for DHTA5, 6 and 7 dissolved in dimethyl sulfoxide and analysed by means of excited state calculations with an time-dependent DFT framework.

CPP 58.3 Wed 17:00 H 0111

photochromic phosphonic-acid diarylethene self-assembled monolayer switches on polar ZnO surfaces — •Qiankun Wang[1], Giovanni Ligorio[1], Valentin Diez-Cabanes[2], David Cornil[2], Björn Kobin[3], Stefan Hecht[3], Jérôme Conil[2], Emil J.W. List-Kratochvil[1], and Norbert Koch[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Laboratory for Chemistry of Novel Materials, University of Mons — [3]Department of Chemistry, Humboldt-Universität zu Berlin

Here, we investigate the interfacial chemical and switching properties of the phosphonic-acid diarylethene (PA-DAE) switch in form of a self-assembled monolayer (SAM) on ZnO(0001) and ZnO(000-1) surfaces by photoelectron spectroscopy and density functional theory calculations. The observed work function increase is attributed to the introduction of a surface dipole; the binding modes of the phosphonic-acid linker were retrieved from the deconvolution of O 1s core level spectra, indicating the formation of mixed bidentate and tridentate binding. The quantification of core level spectra supports the picture of a densely packed SAM on both ZnO surfaces. Upon illumination with ultraviolet and visible light, respectively, we observe a 0.7 eV energy level shift at the onset of the highest occupied molecular orbital (HOMO) level of the PA-DAE molecules. This can further on be used to reversibly switch the energy level alignment at the ZnO/PA-DAE interface in device structures.

CPP 58.4 Wed 17:15 H 0111

Investigation of sputter deposited nanostructured alloy films on polymer surfaces — Niko Carstens[1], Alexander Hinz[1], Oleksandr Polonskyi[1], •Thomas Strunskus[1], Matthias Schwartzkopf[2], Pallavi Pandit[2], Andre Rothkirch[2], Franziska Löhrer[3], Volker Körstgens[3], Simon Schaper[3], Peter Müller-Buschbaum[3], Stephan Roth[2], and Franz Faupel[1] — [1]Chair for Multicomponent Materials, CAU Kiel, 24143 Kiel — [2]DESY, 22607 Hamburg — [3]Physcis Department, TU Munich, 85748 Garching

The fabrication of functional materials with tailored plasmonic properties gained much interest in recent years. Vapor phase deposition techniques like sputtering are an attractive approach to produce self-assembled nanostructured films which exhibit plasmonic activity when the effective thickness is under the percolation threshold. As the local surface plasmon resonance can be tuned by the composition, alloy films are of special interest. In this study, the growth of miscible (AuAg) and immiscible (CuAg) systems on different polymer surfaces (PS and PMMA) by magnetron sputtering has been investigated. The correlation between optical properties and the stage of film growth was examined during deposition by means of in-situ reflection UV-Vis spectroscopy as well as time resolved GIWAXS and GISAXS investigations [1,2]. In addition, SEM investigations as well as ex-situ transmission UV-Vis spectroscopy were performed after film deposition.

[1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 9, 5629 (2017), [2] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015).

CPP 58.5 Wed 17:30 H 0111

Anomalous Roughness Evolution of Organic Mixed Films — •Alexander Hinderhofer, Jan Hagenlocher, Martin Oettel, and Frank Schreiber — Institute of Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

The surface morphology and roughness of thin films and crystals depend on competing mechanisms, which either roughen or smooth the film surface during growth. Important roughening mechanisms, are kinetic roughening based on shot noise and roughening due to mound growth, which is facilitated by reduced interlayer transport, often associated with a step edge. While these issues have been well studied for growth of simple atomic species, comparatively little is known about organic systems. These are expected to exhibit a fundamentally different growth behavior, due to their different interactions (van-der-Waals) and thus different response to strain and due to their internal degrees of freedom.

We use in situ x-ray reflectivity and complementary atomic force microscopy to monitor crystallinity and roughness evolution during growth of organic binary mixtures of several compounds, i.e. pentacene (PEN), perfluoropentacene (PFP), diindenoperylene (DIP) fullerene (C60). A general trend of reduced roughness in the mixed films compared to the pure materials is observed. We will discuss this roughness evolution in relationship to the in-plane crystallinity of the thin films and will show that the growth behavior can be rationalized by a, compared to homoepitaxy, lowered step edge barrier for lower in-plane crystallinity.

CPP 58.6 Wed 17:45 H 0111

Grain boundaries and charge carrier diffusion in large crystal MAPI thin films — •Richard Ciesielski[1], Frank Schäfer[1], Nicolai Hartmann[1], Nadja Giesbrecht[1], Thomas Bein[1], Pablo Docampo[2], and Achim Hartschuh[1] — [1]Department Chemie und Center for Nanoscience (CeNS), LMU München, Deutschland — [2]School of Electrical and Electronic Engineering, Newcastle University, United Kingdom

Micro- and nanocrystalline methyl-ammonium lead-iodide (MAPI)-based thin film solar cells today reach power conversion efficiencies of up to 20%. We investigate the impact of grain boundaries on charge carrier transport in large crystal MAPI thin films using time-resolved photoluminescence (PL) microscopy and numerical model calculations. While long-ranged diffusive charge carrier transport is observed within single crystals, no transport occurs across the grain boundaries. The observed PL transients are found to crucially depend on the microscopic geometry of the crystal and the point of observation. Our experimental results show no quenching or additional loss channels due to grain boundaries for the studied material, which thus do not negatively effect the performance of derived thin film devices.

CPP 58.7 Wed 18:00 H 0111

Nanoporous thin films of organic semiconductors for gas sensing applications — •Jean-Nicolas Tisserant, Wolfgang Kowalsky, and Robert Lovrincic — TU Braunschweig, Institut für Hochfrequenztechnik c/o InnovationLab, Speyerer Str. 4 69115 Heidelberg

Organic semiconducting devices could find applications in high added-value products such as efficient sensors for the detection of toxic gases.(1) Nanoporous morphologies are particularly interesting in this scope because they offer enhanced interfacial areas compared to the corresponding planar materials. Processes such as the diffusion of an analyte molecule to the active area of a gas sensor (2) may thus be improved proportionally to the amount of interface added. We propose to use nanoporous thin films of semiconductors in an organic field-effect transistor (OFET) for sensing of an endocrine disruptor in air. In the strategy that we follow, organic semiconducting molecules were self-assembled into nanoporous 2D films following a recently developed method.(3,4) These films were biased in an OFET configuration to build an indirect sensor in which the non-covalent interaction between a sensing dielectric and the target molecule modifies the electrical characteristics of the transistor.

References: (1)Zhang, C., Chen, P. & Hu, W. Chem. Soc. Rev. 44, 2087-2107 (2015); (2)Zhang, F., Qu, G., Mohammadi, E., Mei, J. & Diao, Y. Adv. Funct. Mater. 27, 17-20 (2017); (3)Tisserant, J. N. et al. RSC Adv. 6, 23141-23147 (2016); (4)Tisserant, J.-N. et al. ACS Appl. Mater. Interfaces 9, 27166-27172 (2017)

CPP 59: Solid-liquid interfaces: Reactions and electrochemisty IV (joint session O/CPP)

Time: Wednesday 16:45–18:00 Location: MA 144

CPP 59.1 Wed 16:45 MA 144

Implicit solvation functionality for surface supercell calculations with the full-potential DFT code FHI-aims — •Jakob Timmermann, Marvin Lechner, Stefan Ringe, Harald Oberhofer, and Karsten Reuter — Technische Universität München

The necessity to account for solvation effects in electrochemical simulations is by now well established. Notwithstanding, explicitly resolving the solvation environment in first-principles based simulations leads to system sizes and sampling requirements that are still often computationally intractable. For this reason, implicit solvation methods, first pioneered over 80 years ago, are currently undergoing a renaissance. One such example is the modified Poisson-Boltzmann implicit solvation functionality that was recently implemented in the numeric atomic orbital based full-potential density-functional theory code FHI-aims [1]. Here, we extent this functionality to periodic boundary conditions, which allows to compute extended solid/liquid interfaces in supercell geometries. The performance and numerical efficiency of the approach is illustrated by computing the potential of zero charge for a range of reference close-packed metal surfaces.

[1] S. Ringe *et al.*, J. Chem. Theory Comput. 12, 4052 (2016).

CPP 59.2 Wed 17:00 MA 144

First-Principles Calculation of Solvent-Mediated Proton Transfer at the TiO_2(110) Surface: Kinetic Barriers and the Effect of Functionals — •Ahmad Agung, Thomas Stecher, Karsten Reuter, and Harald Oberhofer — Technische Universität München

To date, a majority of theoretical studies of (photo-)electrochemical surface reactions focuses on their thermodynamic feasibility. Only recently an ab initio molecular dyamics (AIMD) approach utilizing QM-MM embedding, explicit solvation and the HSE06 hybrid functional was applied to determine the kinetic barrier of H_2O dissociation on a rutile TiO_2(110) surface [1]. Despite advanced sampling techniques and a comparatively small QM region, the use of the hybrid functional rendered these simulations computationally extremely expensive. To this end, we assess in how much generalized-gradient approximation (GGA) functionals can be employed to reduce the computational cost. Not too surprisingly, we find the inferior GGA energetics to yield a significantly different reaction barrier, when directly evaluating GGA-based AIMD trajectories. We therefore assess in how much these GGA trajectories yield at least an appropriate sampling of phase space, thereby offering computational savings by restricting the expensive hybrid level calculations to snapshots along these trajectories.

[1] T. Stecher, K. Reuter and H. Oberhofer, Phys. Rev. Lett. 117, 276001 (2016).

CPP 59.3 Wed 17:15 MA 144

Beyond Catalyst Screening for Electrocatalytic Materials – Importance of Active Site Structure, Mechanism, and Kinetics for the OER on Transition Metal Oxides — •Craig Plaisance, Simeon Beinlich, and Karsten Reuter — Technische Universität München, Germany

Over the past decade or so, the computational design of catalysts for electrochemical reactions has been dominated by an approach in which the catalytic performance of a material is quickly estimated by calculating the values of one or two atomic-level descriptors, typically binding energies of key intermediates on a low index surface of the material. While this approach allows for rapid screening of a vast number of catalyst materials and has indeed identified improved catalysts in several cases, it is based on rather drastic assumptions and can thus only give a rough estimate of catalytic performance. This talk examines the suitability of the descriptor-based screening approach for the OER on doped 3d transition metal oxides, a promising class of earth-abundant materials for catalyzing this reaction. Specifically, we examine whether or not the scaling and Bronsted-Evans-Polanyi relations on which the screening approach is based are robust with respect to changes in the geometry of the active site and the mechanism. We also address whether or not it is necessary to consider the kinetics of certain reaction steps in addition to the thermodynamics. In the end, we conclude that perhaps a more detailed understanding of the quantum chemical properties controlling electrocatalytic performance is needed in order to rationally design an optimal active site.

CPP 59.4 Wed 17:30 MA 144

Band alignment at semiconductor/water interfaces using explicit and implicit descriptions for liquid water — •Nicolas Hörmann[1], Zhendong Guo[2], Francesco Ambrosio[2], Oliviero Andreussi[1], Alfredo Pasquarello[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials (THEOS) and MARVEL, EPFL, Lausanne, Switzerland — [2]Chair of Atomic Scale Simulations (CSEA) and MARVEL, EPFL, Lausanne, Switzerland

We compare the band alignment of several semiconductor/water interfaces for GaAs, GaP, CdS and TiO2 as determined from explicit water ab-initio molecular dynamics simulations based on density functional theory (DFT) to results obtained within a DFT + implicit solvation model (SCCS) [1] as implemented in ENVIRON. It has been demonstrated that solvation effects are an important ingredient to describe the interface energetics in electrochemical systems adequately [2,3], however, it is still unclear how the choice of the explicit water molecules included affects the computational results. This work will allow us to estimate the expected errors of using implicit solvation models, with and without thermodynamic sampling and can serve as a guideline for the amount of interfacial water that should be treated quantum mechanically. [1] O. Andreussi, et al., J. Chem. Phys. 136, 064102 (2012); [2] L. Sementa, et al., Catal. Sci. Technol., 6, 6901-6909 (2016); [3] J. Huang , N. Hörmann, et al. submitted to Nature Materials (2017), under review

CPP 59.5 Wed 17:45 MA 144

On the enhanced self-dissociation of water by bidimensional nanoconfinement — •Daniel Muñoz-Santiburcio[1,2] and Dominik Marx[2] — [1]CIC nanoGUNE, Tolosa Hiribidea 76, 20018

San Sebastián, Spain — [2]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany

Nanoconfined liquids present strikingly different properties compared to the bulk regime. Water in particular is the subject of intense investigation, and in previous works we described how nanoconfinement affects the mechanisms and energetics of chemical reactions therein [1] and also the peculiar differences between the structural diffusion mechanism of H^+(aq) and OH^-(aq) compared to the bulk [2,3]. Now, we present interesting results of advanced *ab initio* simulations which show how bidimensional nanoconfinement enhances one of the most important reactions in water, namely the self-dissociation of H_2O(aq) into H^+(aq) and OH^-(aq) [4]. This surprising feature goes hand in hand with the enhancement of the parallel component of the dielectric constant tensor of the nanoconfined water layer.

[1] D. Muñoz-Santiburcio and D. Marx, *Chem. Sci.* 8 (5), 3444-3452 (2017).

[2] D. Muñoz-Santiburcio and D. Marx, *Nat. Commun.* 7, 12625 (2016)

[3] D. Muñoz-Santiburcio, C. Wittekindt and D. Marx, *Nat. Commun.* 4, 2349 (2013)

[4] D. Muñoz-Santiburcio and D. Marx, *Phys. Rev. Lett.* 119, 056002 (2017).

CPP 60: Polymer and Molecular Dynamics I

Time: Wednesday 17:00–17:30 Location: C 264

CPP 60.1 Wed 17:00 C 264

Molecular Mobility and Physical Aging of Polymers with Intrinsic Microporosity (PIMs) as Revealed by Dielectric Spectroscopy — •Huajie Yin, Nora Konnertz, Martin Böhning, and Andreas Schönhals — Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin, Germany

Polymeric membranes represent a cost- and energy- efficient solution for gas separation. Recently polymers of intrinsic microporosity (PIMs) outperform many conventional dense polymers by high permeability and appealing selectivity. However, this novel class of glassy polymers are prone to pronounced physical aging. The initial microporous structures approach a denser state via local chain rearrangements, leading to a dramatic reduction in the gas permeability. For the first time, dielectric spectroscopy with state-of-the-art high-resolution analyzers was employed to investigate the molecular mobility and physical aging of various representative PIMs with a systematic change in chain rigidity. The dielectric behavior of the polymeric films was measured by isothermal frequency scans during the different heating cycles in a broad temperature range. Structural relaxation of the films was found during the measurements. Multiple dielectric processes following Arrhenius behavior were observed for the investigated polymers. Moreover, they all showed conductivity in the glassy state. The significant increase in the conductivity with increasing temperature is explained in terms of the formation of local intermolecular agglomerated structures due to interaction of π-electrons in aromatic moieties of the polymer backbone.

CPP 60.2 Wed 17:15 C 264

First Clear-cut Experimental Evidence for A Glass Transition in Polymers of Intrinsic Microporosity (PIMs) — •Huajie Yin[1], Yeong Zen Chua[2], Bin Yang[2], Christoph Schick[2], Martin Böhning[1], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — [2]University of Rostock, Institute of Physics and Competence Center CALOR, Albert-Einstein-Str. 23-24, 18059 Rostock, Germany

Polymers with intrinsic microporosity (PIMs) represent a novel innovative class of materials with great potential in several applications from high-performance gas separation membranes to electronic devices. Microporosity with BET surface areas > 700 m2/g is due to their rigid structure resulting in limited molecular mobility. Up to now no glass transition temperature (Tg) could be detected before degradation. Therefore, it is important to clarify whether PIMs undergo a glass transition. Decoupling the time scales responsible for the glass transition and decomposition is a reliable strategy. This was achieved by employing fast scanning calorimetry (FSC) based on a chip sensor, which is capable to heat and cool a small amount of sample with extremely high heating/cooling rate of many thousands of Kelvin per second. For the first time, Tg values of two archetypal representatives of PIMs: PIM-1 and PIM-EA-TB were determined. FSC provides clear-cut experimental evidence of the glass transition of PIM-1 with a Tg of 442 °C and PIM-EA-TB with a Tg of 404 °C at a heating rate of 30,000 K/s.

CPP 61: Focus: Fundamental Physics of Perovskites II - organized by Lukas Schmidt-Mende and Vladimir Dyakonov

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

Topical Talk CPP 61.1 Thu 9:30 C 130

Approaching the Shockley-Queisser Limit with Interface Control in Halide Perovskites — •David Ginger — University of Washington, Seattle, USA

Although remarkable gains in performance have been demonstrated for halide perovskite semiconductors, most current perovskite solar cells are still limited by non-radiative recombination losses. In this talk, I will focus on uncovering and eliminating these loss processes. Experiments suggests that electrical heterogeneities in both the perovskite active layer, as well as the perovskite/electrode interface, affect carrier diffusion and non-radiative recombination processes within perovskite solar cells. I will describe both confocal and conductive atomic force microscopy (cAFM) to explore the role of heterogeneities and grain boundaries on lateral carrier transport, and will demonstrate varying degrees of grain boundary opacity to carrier transport depending on the structure. We will also discuss both ligand exchange and cation exchange experiments in the context of tailoring the surface properties of halide perovskite thin films. We show that with controlled passivation of the perovskite surfaces we are able to obtain carrier lifetimes and PL intensities in solution-processed thin films that rival those in the best single crystals, achieving over 90% PL internal quantum efficiency and quasi-Fermi level splittings that exceed 96% of the Shockley-Queisser limit under illumination. Combining these results with experiments demonstrating contact-induced losses in many common perovskite architectures, we then explore new contact materials and their potential for increased efficiency.

CPP 61.2 Thu 10:00 C 130

Active Materials and interfaces for stable perovskite solar cells — •Antonio Abate — Helmholtz-Zentrum Berlin für Materialien und Energie

Organic-inorganic perovskites are quickly overrunning research activities in new materials for cost-effective and high-efficiency photovoltaic technologies. Since the first demonstration from Kojima and coworkers in 2009, several perovskite-based solar cells have been reported and certified with rapidly improving power conversion efficiency. Recent reports demonstrate that perovskites can compete with the most efficient inorganic materials, while they still allow processing from solution as a potential advantage to deliver a cost-effective solar technology. Compare to the impressive progress in power conversion efficiency, stability studies are rather weak and often controversial. An intrinsic complication comes from the fact that the stability of perovskite solar cells is strongly affected by any small difference in the device architecture, preparation procedure, materials composition and testing procedure. In the present talk, we will focus on the stability of perovskite solar cells in working condition. We will discuss a measuring protocol to extract reliable and reproducible ageing data. We will present new materials and preparation procedures, which improve the device lifetime without giving up on high power conversion efficiency.

CPP 61.3 Thu 10:15 C 130

Visualizing and suppressing interfacial recombination in high efficiency large area pin-perovskite solar cells — •Martin Stolterfoht[1], Christian M. Wolff[1], Shanshan Zhang[1,2], José A. Márquez Prieto[3], Charles J. Hages[3], Daniel Rothhardt[1], Thomas Unold[3], Steve Albrecht[4], Paul L. Burn[2], Paul Meredith[5], and Dieter Neher[1] — [1]University of Potsdam, Potsdam-Golm, Germany — [2]The University of Queensland, Brisbane, Australia — [3]Helmholtz-Zentrum-Berlin, Berlin, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [5]Swansea University, Swansea, United Kingdom

The current generation of perovskite solar cells (PSCs) is predominantly limited by non-radiative recombination, either through trap-assisted recombination in the absorber layer, or via minority carrier recombination at the interface to the transport layers. Using transient and absolute photoluminescence imaging we are able to visualize all relevant non-radiative recombination pathways in planar pin-type PSCs. We find significant quasi-Fermi level splitting losses (135 meV) in the perovskite bulk, while interface recombination results in an additional energy loss of 80 meV at each individual interface. These losses define the open-circuit voltage of the complete cell. Inserting ultrathin interlayers between the perovskite and transport layers allows substantial reduction of these interfacial losses at both the p-and-n-contacts. Using this knowledge and approach, we demonstrate stable 1 cm2 PSCs surpassing 20% efficiency (19.83% certified) with record fill factor (> 81%), high V_OC (1.17V) and near unity manufacturing yield.

CPP 61.4 Thu 10:30 C 130

Passivating perovskite surfaces by mixtures of PEDOT and dopant-free Spiro-OMeTAD — •L. Kegelmann[1], C. M. Wolff[2], J. A. Márquez Prieto[1], P. Tockhorn[1], T. Unold[1], D. Neher[2], B. Rech[1], and S. Albrecht[1] — [1]Helmholtz-Zentrum Berlin, Berlin, Germany — [2]University of Potsdam, Institute of Physics and Astronomy, Potsdam, Germany

Perovskite solar cells have achieved efficiencies above 22% within few years. By now, the device parameter with the largest potential for further improvements is the open circuit voltage (Voc), which is mainly limited by recombination losses at the interfaces. Here, a poly(3,4-ethylenedioxythiophene) (PEDOT) layer doped with sulfonated copolymers is utilized as a hole selective contact (HSC) on top of perovskite absorbers. Transient photoluminescence (PL) and steady-state PL quantum yield measurements reveal longer charge carrier lifetimes and larger quasi-fermi level splitting for perovskite films after the PEDOT is deposited. PEDOT thin films therefore seem to suppress charge carrier recombination at the perovskite surface. By blending undoped Spiro-OMeTAD into the PEDOT dispersion, the surface energetics of the resulting films are shifted to larger ionisation energies as measured by photoelectron spectroscopy and the quasi-fermi level splitting is further enhanced. As a result, perovskite solar cells with mixtures of PEDOT and Spiro-OMeTAD as HSC achieve high Voc values above 1.15 V and stabilized efficiencies over 16%. This exceeds the Voc of reference devices with either doped Spiro-OMeTAD or pure PEDOT as HSC.

CPP 61.5 Thu 10:45 C 130

Revealing the impact of Rubidium and Cesium on the electronic trap landscape of mixed cation perovskite solar cells via thermally stimulated current — •Philipp Rieder[1], Yinghong Hu[3], Alexander Hufnagel[3], Meltem Aygüler[3], Michiel Petrus[3], Pablo Docampo[4], Kristofer Tvingstedt[1], Andreas Baumann[2], Thomas Bein[3], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg — [3]Department of Chemistry and Center for NanoScience (CeNS), LMU Munich, 81377 Munich — [4]Physics Department, Newcastle University, Newcastle upon Tyne, NE1 7RU, United Kingdom

In the last years, mixed cation and halide organo-lead perovskite has established itself as the working horse in the perovskite community, due its improved crystallization behavior and therefore reproducible high power conversion efficiencies (PCE) achieved in various solar cell configurations. Recently, this so-called "FAMA" perovskite, whereas methylammonium (MA) and bromide is used to stabilize the crystal structure of formamidinium (FA) lead iodide perovksite, could be further improved by the introduction of small amounts of Rb as well as Cs, boosting the device PCE up to 21.6%, while additionally enhancing the long-term stability. Here, we use thermally stimulated current (TSC) spectroscopy to study the beneficial impact of Cs and/or Rb on the FAMA crystal lattice by directly probing the electronic trap landscape in what has been come to be known as triple and quadruple cation perovskite solar cells.

15 min. break

Topical Talk CPP 61.6 Thu 11:15 C 130

Understanding Hysteresis in Perovskite Solar Cells — •Stefan A.L. Weber[1,2], Ilka M. Hermes[1], Niklas M. Budinger[1,2], Wolfgang Tress[3], Anders Hagfeldt[3], Michael Graetzel[3], and Rüdiger Berger[1] — [1]MPI for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Johannes Gutenberg University, Department of Physics, Staudingerweg 10, 55128 Mainz, Germany. — [3]Laboratory of Photomolecular Science, Institute of Chemical Sciences and Engineering, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland.

We explain the underlying mechanism of hysteresis in a hybrid lead-halide perovskite solar cell by measuring and numerically calculating the dynamics of the charge distribution in an operating device. The origin, magnitude and the dynamics of the charge re-distribution processes that are responsible for hysteresis in the device are still not understood. We developed a method based on Kelvin probe force microscopy that enables mapping charge re-distribution in an operating device upon a voltage- or light pulse with sub-millisecond resolution. A combination of an asymmetric ion migration and the formation of a surface dipole at the anode shielded the electric field in the perovskite layer within 10 ms after applying a forward voltage to the device. After switching off the voltage, the anode surface dipole created a reverse electric field in the cell that lasted for up to 500 ms. This reverse electric field increases charge carrier extraction and thereby directly explains higher photocurrents during reverse bias scans.

CPP 61.7 Thu 11:45 C 130

Recombination in Perovksite Solar Cells — •Wolfgang Tress — Laboratory for Photonics and Interfaces, Institute of Chemical Sciences and Engineering, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Solar cells based on metal halide perovskite absorber materials are about to emerge as a high-efficiency photovoltaic technology. At the same time, they are suitable for high-throughput manufacturing characterized by a low energy input and abundant low-cost materials. However, a further optimization of their efficiency, stability and reliability demands for a more detailed optoelectronic characterization and understanding of losses including their evolution with time.

In this work, we analyze perovskite solar cells with different architectures (planar, mesoporous, HTL-free), employing temperature dependent measurements (current-voltage, light intensity, electroluminescence) of the ideality factor to identify dominating recombination processes that limit the open-circuit voltage (V_{oc}). We find that in thoroughly-optimized, high-V_{oc} (> 1.2 V) devices recombination prevails through defects in the perovskite. On the other hand, irreversible degradation at elevated temperature is caused by the introduction of broad tail states originating from an external source (e.g. metal electrode). Light-soaking is another effect decreasing performance, though reversibly. Based on FTPS measurements, this degradation is attributed to the generation of surface defects becoming a new source of non-radiative recombination.

CPP 61.8 Thu 12:00 C 130

Long-range charge extraction in quasi-interdigitated back-contact hybrid perovskite solar cells — •Gregory Tainter[1,2], Maximilian Hoerantner[3], Luis Miguel Pazos-Outón[1], Suhas Mahesh[3], Richard Friend[1], Henry Snaith[3], Hannah Joyce[2], and Felix Deschler[1] — [1]Cavendish Laboratory, Department of Physics, University of Cambridge, JJ Thomson Avenue, Cambridge CB3 0HE, UK — [2]Department of Engineering, University of Cambridge, Cambridge CB3 0FA, UK — [3]Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, UK.

Understanding charge extraction in photovoltaic devices is critical to engineering practical applications. Here we study individual charge extraction and charge recombination via scanning photocurrent measurements on quasi-interdigitated back-contact (QIBC) hybrid perovskite devices. Lateral separation of carriers is achieved via excitation over charge-selective electrodes and non-ambipolar charge transport is characterised. We model charge carrier diffusion and report electron and hole diffusion constants in operating QIBC devices. A large fraction of holes and electrons are found to propagate through multiple grain boundaries, and carrier recombination is reduced due to charge separation as indicated by our diffusion model.

CPP 61.9 Thu 12:15 C 130

Surface State Density Determines the Energy Level Alignment at Hybrid Perovskite/Electron Acceptor Interfaces — •Fengshuo Zu[1,2], Patrick Amsalem[1], Maryline Ralaiarisoa[1,2], Thorsten Schultz[1], Raphael Schlesinger[1,2], and Norbert Koch[1,2] — [1]Institut für Physik, HU Berlin — [2]HZB, 12489 Berlin

Substantial variations of the surface electronic structure and thus conflicting energetics at interfaces between hybrid perovskites and charge transport layers can be found in literature. In an attempt to unravel the origin of these variations, we demonstrate that donor-like surface states stemming from reduced lead (Pb0) directly impact the energy level alignment at perovskite and molecular electron acceptor interfaces, using photoelectron spectroscopy. When forming the interfaces, it is found that electron transfer from surface states to acceptor molecules occurs, leading to a strong decrease in the density of ionized surface states. As a consequence, for perovskites with low surface state density, the initial band bending at the pristine perovskite surface can be flattened upon interface formation. In contrast, for perovskites with a high surface state density, the Fermi-level is strongly pinned at the conduction band edge and only minor changes in surface band bending are observed upon acceptor deposition. Consequently, depending on the initial surface state density, very different interface energy level alignment situations (variations over 0.5 eV) are demonstrated and rationalized. Our findings help explaining the rather dissimilar reported energy levels at interfaces and refining our understanding of the operating principles in devices comprising this material.

CPP 61.10 Thu 12:30 C 130

Self-assembled Monolayers Enhance the Stability and Efficiency of p-i-n Perovskite Solar Cells — •Christian Wolff[1], Martin Stolterfoht[1], Yohai Amir[1], Antonio Abate[2], and Dieter Neher[1] — [1]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, 14476, DE — [2]Institut für Silizium-Photovoltaik, Helmholtz-Zentrum Berlin für Materialien und Energie,12489 Berlin, DE

Perovskite solar cells with all-organic transport layers have shown efficiencies rivalling their counterparts that employ high temperature treated inorganic transport layers [1,2,3]. One of the main issues associated with perovskite solar cells is their instability, in particular towards long periods of illumination or moisture and closely related the lack of control of the nature and electronic structure of the interface between the active perovskite and the adjacent transport layers. In this contribution we show that in p-i-n cells interjection of a self-assembling monolayer between the perovskite and the adjacent electron transport layer allows us to produce solar cells with efficiencies above 20% on small areas (6 mm2) as well as 1 cm2 with almost no loss by scaling. Importantly, these cells exhibit enhanced resilience towards heat and light illumination as exemplary shown by keeping the solar cells at 85°C under full load (MPP, simulated 1 sun illumination) for 250h without appreciable efficiency loss.

[1] Wolff et al., Adv.Mater., 2017, 29, 1700159 [2] Stolterfoht et al., Energy and Environ. Sci., 2017, 10, 1530-1539 [3] Zheng et al., Nat. Energy, 2017, 2, 17102

CPP 61.11 Thu 12:45 C 130

Structure and electronic properties characterization of $CH_3NH_3PbI_{3-x}Cl_x$ mixed halide perovskite films upon massive solvents exposure — •Maryline Ralaiarisoa[1], Yerila Rodriguez[2], Ingo Salzmann[1], Lidice Vaillant[2], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik & IRIS Adlershof — [2]Physics Faculty, University of Havana

We combined photoelectron spectroscopy (PES), grazing incidence X-ray diffraction, UV-Vis absorption spectroscopy, and atomic force microscopy to characterize the effect of massive solvent exposure on $CH_3NH_3PbI_{3-x}Cl_x$ mixed halide perovskite films. We selected solvents that can potentially be used to solution-deposit organic charge transport layers on top of the perovskite: water, dimethylformamide (DMF), chloroform (CF), and chlorobenzene (CB). Water and DMF instantly dissolved the perovskite films. Particularly, water degraded the perovskite film into a yellow PbI_2 film, along with the generation of reduced Pb^0 precipitates. Furthermore, PES results indicate the presence of methyl ammonium or related compounds even after water dissolution. Although the crystal structure and morphology of perovskite films were preserved upon CF and CB exposure, the valence band and therefore the electronic properties of the films were strongly altered, as a result of surface state modifications. In fact, the film surfaces become less n-type upon exposure, possibly due to a reduction of surface Pb^0-species. Thus, the use of CB and CF for solution deposition of organic charge transport layers is possible, but can already substantially modify the perovskite properties at the interface.

CPP 62: Charged Soft Matter, Polyelectrolytes and Ionic Liquids III

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

CPP 62.1 Thu 9:30 C 243

Hydrophobicity/hydrophilicity altered by light: A case study of photosensitive cationic azobenzene surfactants — Maria Montagna[1] and •Olga Guskova[1,2] — [1]Institute Theory of Polymers, Leibniz Institute of Polymer Research Dresden, Hohe Straße 6, 01069, Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), Technische Universität Dresden 01062, Dresden, Germany

In this work we present a computational study of the photosensitive cationic surfactants with a conventional trimethylammonium or pH-sensitive polyamine hydrophilic head and the azobenzene containing hydrophobic tail immersed in water. The azobenzene molecules are known to undergo a reversible tran-cis-trans isomerization upon the UV-visible light irradiation. Combining the density functional theory and the atomistic molecular dynamics simulations, the structural and the hydration properties of the trans- and the cis-isomers are investigated. We establish and quantify the correlations of the isomerization state of the surfactant tail and the molecular hydrophilicity/hydrophobicity altered by light. Furthermore, our findings are compared with the experimental data [1] and the predictions of the thermodynamic theory [2] on the self-assembly of photosensitive cationic azobenzene surfactants incorporated in soft nano-objects. This work was supported by DFG (Project GU 1510/3-1).

[1] S. Schimka et al. Phys. Chem. Chem. Phys. 2017, 19, 108.

[2] A.M. Rumyantsev et al. Macromolecules 2014, 47, 5388.

CPP 62.2 Thu 9:45 C 243

Interfaces in fluids of ionic liquid crystals — •Hendrik Bartsch[1,2], Markus Bier[1,2], and Siegfried Dietrich[1,2] — [1]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Deutschland — [2]Universität Stuttgart, Stuttgart, Deutschland

Ionic liquid crystals are 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. Recently, for such an ionic liquid crystal system a new type of smectic-A bulk structure could be observed, the smectic layer spacing of which is significantly larger than that of the ordinary smectic-A phase [HB et al, 2017, J. Phys.: Condens. Matter 29 464002]. Moreover, unlike the ordinary smectic-A phase it shows alternating layers of particles parallel to the layer normal and oriented perpendicular to it. This finding stresses that ionic liquid crystals exhibit distinct structural and orientational behavior. In particular in inhomogeneous systems, e.g., an electrolyte in the vicinity of an electrode or interfaces between bulk phases, these properties are very important and they are expected to affect the interfacial phenomena of these materials crucially.

In this talk, we report on new findings, obtained within classical density functional theory, concerning the fluid structure and molecular orientations at a free interface of coexisting bulk phases. We discuss and compare the density and orientational order parameter profiles for different kinds of the liquid-smectic phase coexistence occurring in ionic liquid crystals and ordinary (uncharged) liquid crystals.

CPP 62.3 Thu 10:00 C 243

Salt and Polymer Dynamics in PPG based Polymer Electrolytes: A ^{1}H and ^{7}Li NMR study — •Manuel Becher, Simon Becker, Lukas Hecht, and Michael Vogel — TU Darmstadt Condensed Matter Physics, Darmstadt, Germany

Facing an increasing need for safe and mechanically stable devices for energy storage, solid-state (lithium)-ion conducting batteries are in the focus of current research. As one of the central components, the electrolyte determines desirable features like high energy density, light weight and high ion conductivity. Polymer electrolytes (salts dissolved in polymers) are already used in portable devices, but suffer from lower electric conductivity as compared to other alternatives. Hence, it is of great interest to enhance the ion diffusivity in the polymer matrix. For this purpose, a fundamental understanding of the transport mechanisms is necessary, but still not available. Here, we focus on amorphous polypropylene glycol (PPG) lithium-salt mixtures, comparing different salts and salt concentrations. We combine several nuclear magnetic resonance (NMR) experiments, namely diffusometry, relaxometry, spectroscopy and exchange studies to ascertain ion and polymer dynamics over a wide range of length and time scales. Selectively investigating cation, anion and polymer host dynamics (^{7}Li, ^{19}F and ^{1}H measurements, respectively) yields a strong correlation between polymer reorientation and ion diffusion. Moreover, we show that the ion transport is strongly affected by a structural inhomogeneity of the mixtures which depends on the solubility of the salts. In this context, we discuss the differences in conductivity of LiClO$_4$ and LiTFSI salts.

CPP 62.4 Thu 10:15 C 243

Force fields for monovalent and divalent metal cations in TIP3P water based on thermodynamic and kinetic properties — •Nadine Schwierz[1] and Shavkat Mamatkulov[2] — [1]Max Planck Institut für Biophysik, Frankfurt, Germany — [2]The Centre of Higher Technologies, Tashkent, Uzbekistan

Metal cations are essential in many vital processes. In order to capture the role of different cations in all-atom molecular dynamics simulations of biological processes, an accurate parametrization is crucial. Here, we develop force field parameters for the metal cations Li+, Na+, K+, Cs+, Mg2+, Ca2+, Sr2+, and Ba2+ in combination with the TIP3P water model that is frequently used in biomolecular simulations. In progressing toward improved force fields, the approach presented here is an extension of previous efforts and allows us simultaneously reproduce thermodynamic and kinetic properties of aqueous solutions. We systematically derive the parameters of the 12-6 Lennard-Jones potential which accurately reproduce the experimental solvation free energy, the activity derivative, and the characteristics of water exchange from the first hydration shell of the metal cations. In order to reproduce all experimental properties, a modification of the Lorentz- Berthelot combination rule is required for Mg2+. Using a balanced set of solution properties, the optimized force field parameters aim to capture the fine differences between distinct metal cations including specific ion binding affinities and the kinetics of cation binding to biologically important anionic groups.

CPP 62.5 Thu 10:30 C 243

structural and transport properties of Li/S battery electrolytes using molecular dynamics simulations — •Chanbum Park[1,2], Matej Kanduč[1], Richard Chudoba[1,2], Arne Ronneburg[1,2], Sebastian Risse[1], Matthias Ballauff[1,2], and Joachim Dzubiella[1,2] — [1]Institut für Weiche Materie und Funktionale Materialien, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Lithium-Sulfur (Li/S) batteries are a promising energy storage device as post lithium-ion battery candidates. Despite the vast experimental and theoretical research on Li/S batteries, practical performance is not yet achieved. Fundamental molecular insights of transport and structure properties of lithium polysulfides in solvents are necessary. We constructed a classical molecular dynamics (MD) computer simulation model of lithium polysulfides (Li$_2$S$_4$, Li$_2$S$_6$ and Li$_2$S$_8$), lithium-bis(trifluoromethane)sulfonimide (LiTFSI), lithium nitrate (LiNO$_3$) and the organic solvents, 1,2-dimethoxyethane (DME) and 1,3-dioxolane (DOL). We benchmarked and validated our simulations by comparing structural and dynamic features with various available experimental reference systems. We discuss the detailed transport and structural properties of Li/S electrolytes. In particular, our study shows how the ionic conductivity which is affected by ion pairing of Li^{+} with counter ions and clustering of polysulfides in Li/S battery electrolytes.

CPP 62.6 Thu 10:45 C 243

Ionic liquid post-treatment of PEDOT:PSS thin films for improvement of thermoelectric properties — •Nitin Saxena, Benjamin Pretzl, Xaver Lamprecht, Lucas Kreuzer, and Peter Müller-Buschbaum — TU München, Phyisk-Department, LS Funktionelle Materialien, 85748 Garching

Thermoelectric devices based on conducting polymers, especially PEDOT:PSS, have attracted great research attention in recent years, mainly focusing on improving electrical conductivities and Seebeck coefficients of thin films. We perform post-treatments of PEDOT:PSS thin films using solutions of different ionic liquids dissolved in THF based on a rational choice of ionic liquids, i.e. keeping the same cation, while varying the anion. This leads to strong implications regarding the thermoelectric properties, especially since Seebeck coefficient and electrical conductivity are increased simultaneously, leading to high power factors of thin films. Spectroscopic methods are used to identify changes in the electronic structure, while x-ray scattering techniques are used to determine changes in the morphology. In addition, temperature-dependent resistivity measurements allow for investigation of changes in the charge transport mechanism upon treatment with ionic liquids.

15 min. break

CPP 62.7 Thu 11:15 C 243

Molecular Mobility and Ionic Conductivity of Ionic Liquid Crystals Forming a Hexagonal Columnar Mesophase — •Arda Yildirim[1], Paulina Szymoniak[1], Kathrin Sentker[2], Martin Butschies[3], Andrea Bühlmeyer[3], Sabine Laschat[3], Patrick Huber[2], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — [2]Institut für Materialphysik und -technologie, Technische Universität Hamburg, Eißendorfer Str. 42, 21073 Hamburg, Germany — [3]Institut für Organische Chemie, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany

For the first time, the molecular mobility of two linear-shaped tetramethylated guanidinium triflates ionic liquid crystals (ILCs) having different length of alkyl chains was investigated by a combination of broadband dielectric spectroscopy (BDS) and specific heat spectroscopy (SHS). SHS was carried out by differential AC-chip calorimetry at higher frequencies and temperature modulated DSC at lower frequencies. These ILCs can form a hexagonal ordered columnar mesophase. Two relaxation processes were found by BDS for both samples. At low temperatures, a γ-processes is observed which is assigned to specific localized fluctuations. At higher temperatures, $\alpha 1$-processes take place. $\alpha 2$-processes were also detected by SHS but with a completely different temperature dependence of the relaxation times. Different molecular assignments of $\alpha 1$- and $\alpha 2$-processes are suggested. At even higher temperatures, conductivity was detected by BDS.

CPP 62.8 Thu 11:30 C 243

Nonlinear Conduction in Ionic Liquids – Insights from Molecular Dynamics Simulations — •Diddo Diddens[1] and Andreas Heuer[1,2] — [1]Helmholtz-Institut Münster, Ionics in Energy Storage (IEK-12), Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany — [2]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany

Ionic liquids (ILs) are promising electrolyte materials for batteries or supercapacitors due to their intrinsically high density of charge carriers and their wide electrochemical stability window. With respect to electrolyte optimization, the ionic conductivity is another important key parameter. In experiments, this quantity is typically measured at rather weak electric fields, at which the conductivity itself is independent of the strength of the applied field. However, nonlinear conduction effects – typically leading to an increase of the ionic conductivity – may come into play at high electric fields [1], which in battery cells usually emerge near electrodes.

In this contribution, we employ nonequilibrium molecular dynamics simulations of ILs in order to characterize the nonlinear conduction mechanism at the molecular level. Special emphasis is put on the interplay of field-induced structural rearrangements and the emergence of nonlinear effects in the conductivity.

[1] L. N. Patro, O. Burghaus, B. Roling, *Phys. Rev. Lett.*, **2016**,

116(18), 185901

CPP 62.9 Thu 11:45 C 243

Charge Transport and Glassy Dynamics in Polymeric Ionic Liquids as studied in its in Inter- and Intramolecular Interactions — •Falk Frenzel[1], Pia Borchert[2], Arthur Markus Anton[1], Veronica Strehmel[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Leipzig, Germany — [2]Hochschule Niederrhein, Krefeld, Germany

Polymeric Ionic Liquids (PILs) are a novel class of materials in which the properties of Ionic Liquids (ILs) are combined with them of polymeric systems. In the present study Broadband Dielectric Spectroscopy (BDS), Fourier Transform Infrared Spectroscopy (FTIR), AC-Chip Calorimetry (ACC) and Differential Scanning Calorimetry (DSC) are employed to analyze the impact of inter- and intramolecular interactions on charge transport and glassy dynamics. By comparing PILs with their low molecular weight counterparts as well as by systematically varying the anion or cation enables one to unravel the mechanism of charge transport and its interplay with glassy dynamics. The detailed findings are in accordance with the model of a dynamic glass transition assisted hopping conduction.

Ref.:

[1] Frenzel, F.; Kremer, F. et al. Springer: Dielectric Properties of Ionic Liquids 2016

[2] Frenzel, F.; Kremer, F. Macromolecules 2017

CPP 62.10 Thu 12:00 C 243

Ionic Liquids in Nano-Confinement: Tuning and Suppressing Their Conduction in Nanoporous Metal-Organic Frameworks — Anemar Bruno Kanj, Rupal Verma, Modan Liu, Julian Helfferich, Wolfgang Wenzel, and •Lars Heinke — Karlsruhe Institute of Technology (KIT), Karlsruhe

Room-temperature ionic liquids (IL) are molten salts of organic molecules and possess outstanding physical and chemical properties. In addition to uses as unique solvents and in catalysis, it may find applications in electronics, sensors and batteries, where the properties under confinement are important. Metal-organic frameworks (MOFs) are nanoporous, crystalline hybrid materials composed of metal ions connected by organic linker molecules.

Here, we investigate the conduction properties of 1-butyl-3-methylimidazolinium bis(trifluoronethylsulfonyl)-imide, referred to as [BMIM][NTf2], ionic liquid under nano-confinement in nanoporous MOFs of type HKUST-1. We use MOFs in form of well-defined, dense films prepared in a layer-by-layer manner, also referred to as SURMOFs.

It was experimentally found that the percentage of pore filling of [BMIM][NTf2] in HKUST-1 has a tremendous impact on the IL conduction properties. The conductivity and ion mobility decreases by three orders of magnitude when the pores of the MOFs are filled. Details of the conduction of IL in the nanopores are unveiled by detailed molecular dynamic (MD) simulations. Mutual pore blockage and transient jamming was found to be responsible for the conductivity drop.

CPP 62.11 Thu 12:15 C 243

Dielectric Spectroscopy on Choline-Chloride Based Deep Eutectic Solvents — •Daniel Reuter, Peter Lunkenheimer, and Alois Loidl — Experimental Physics V, University of Augsburg, Germany

Deep eutectic solvents (DES) are a promising new class of ionic liquid analogues [1]. Via mixing of two solid materials in eutectic composition, a DES liquid phase is obtained that is characterized by its low melting point compared to its individual constituents. Prominent examples are the mixtures of Choline Chloride (ChCl) with various hydrogen bound donors like, e.g., glycerol [2]. In this talk, we present dielectric spectroscopy data of three ChCl based DES in a broad frequency and temperature range. Especially, we investigate the so far widely neglected molecular reorientational dynamics and its correlation to the ionic conductivity. Here, our findings provide valuable information on molecular and ion diffusion in DES.

[1] E. Smith, A. Abbott, and K. Ryder, Chem. Rev. **114**, 11060 (2014). [2] D. Wagle, H. Zhao, and G. Baker, Acc. Chem. Res. **47**, 2299 (2014).

CPP 62.12 Thu 12:30 C 243

Interfacial Water Structure and Properties of Non-Equilibrium CTAB/Polyelectrolyte Mixtures with different Molecular Weights — •Felix Schulze-Zachau and Björn Braunschweig — Institute of Physical Chemistry, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Mixtures of CTAB and 0.1 mM poly(sodium 4-styrenesulfonate) (NaPSS) with different molecular weights (MWs) from 10 kDa to 1 MDa were studied in the bulk with turbidity and ζ-potential measurements, while vibrational SFG spectroscopy and tensiometry provided information on the molecular structure of air/water interfaces. We also relate the molecular structure and the charging state of the interface to the stability and the structure of macroscopic foam. We propose that mostly negatively charged and well-solvated complexes are formed in the bulk at CTAB concentrations below 75 μM. This is corroborated by the negligible turbidity and the ζ-potential of the mixtures. Increasing the CTAB concentration to stoichiometric bulk mixing ratio yields complexes with negligible net charges. These complexes tend to aggregate and adsorb at the interface. The turbidity maximum is indicative to bulk aggregation and shifts with increasing MW to higher CTAB concentrations. The non-equilibrium nature of these mixtures is obvious from the surface tension kinetics which show two adsorption processes of free CTAB and aggregates. Above a threshold concentration, interfaces are dominated by free CTAB while positively charged complexes are well solvated in the bulk. This yields wet foams and is confirmed by measurements with deuterated CTAB.

CPP 62.13 Thu 12:45 C 243

How to tune the surface forces of PDADMA terminated polyelectrolyte multilayers — •Heba Soker Mohamad, Sven Neuber, and Christiane A. Helm — Institut für Physik, Uni. Greifswald, Felix-Hausdorff-Str. 6 17489 Greifswald

Films built from the Poly (styrenesulfonate) (PSS) and poly (diallylmethylammonium) (PDADMA) in 0.1 Mol/L NaCl are investigated. Colloid probe measurements show that PDADMA-terminated surfaces are always positively charged. They are flat if the film consists of few layers. By increasing the number of layers, steric forces due to chains protruding into solution are observed. The PDADMA chains scale as polyelectrolyte brushes and collapse at 1 M NaCl. If the top layers contain an excess of PDADMA monomers neutralized by Cl- ions, at salt concentrations larger than 1 M NaCl again brushes form. Also NaCl penetrates into the film, breaks up ionic monomer-monomer bonds and causes irreversible changes. Concluding, surface forces of polyelectrolyte multilayer can be controlled by preparation and post-preparation treatment.

CPP 63: Polymer and Molecular Dynamics II

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

CPP 63.1 Thu 9:30 C 264

Local dynamics in polyelectrolyte multilayers and complexes — •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str 6, 01069 Dresden, Germany

Relaxation NMR can measure molecular mobility over a wide range of correlation times. The longitudinal relaxation time in the rotating frame (T1rho) is ideally suited for molecular chain motion in the range kiloHertz. If is detected in solid-state NMR with chemical shift resolution, the mobility can be attributed to individual functional groups and thus the mobility of polycation and polyanion in the multilayers or complexes are separated.Thsu dynamic heterogeneity between PDADMAC and PSS in multilayers formed from high-salt solutions has been observed. This is compared to the local mobility in polyelectrolyte complexes formed from the same solutions and those formed from salt-free solutions, exhibiting more homogeneous mobility.

CPP 63.2 Thu 9:45 C 264

Enhancing the Lithium Ion Transport in Polymer Electrolytes – Plasticization and Shuttling — •Diddo Diddens[1] and Andreas Heuer[1,2] — [1]Helmholtz-Institut Münster, Ionics in Energy Storage (IEK-12), Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany — [2]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany

Solid polymer electrolytes consist of a salt dissolved in an amorphous polymer matrix, resulting in mechanically stable and flexible ion conductors. However, at ambient temperatures, their conductivity is still too low for an efficient use in modern energy storages. To overcome this deficiency, the addition of a low-molecular additive such as an ionic liquid (IL) has been proposed. We demonstrate by molecular dynamics simulations that the way in which the IL enhances the lithium mobility can in principle be twofold: First, the IL can act as a plasticizer, enhancing the dynamics of the polymer segments and thus also the motion of the attached lithium ions [1,2], and second, for IL molecules that directly coordinate to the lithium ions, the IL may serve as a *shuttle* detaching the lithium ions from the slow polymer chains [3], resulting in a much larger enhancement. In this contribution, we screen a large range of electrolyte compositions to identify molar ratios facilitating fast ion transport to serve as a guideline for electrolyte optimization.
[1] D. Diddens, A. Heuer, *ACS Macro Lett.*, **2013**, 2(4), 322-326
[2] D. Diddens, A. Heuer, *J. Phys. Chem. B*, **2014**, 118(4), 1113-1125
[3] D. Diddens *et al.*, *J. Electrochem. Soc.*, **2017**, 164(11), E3225

CPP 63.3 Thu 10:00 C 264

Probing intramolecular energy transfer rates on the single molecule level — •Jakob Schedlbauer[1], Philipp Wilhelm[1], Florian Hinderer[2], Sigurd Höger[2], Jan Vogelsang[1], and John M. Lupton[1] — [1]Universität Regensburg, Universitätsstr. 31, 93053 Regensburg, Germany — [2]Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Efficient excitation energy transfer (EET) is a key process in organic photovoltaic devices as well as in natural light harvesting complexes. Single molecule spectroscopy (SMS) has proved itself to be a powerful technique to probe the interactions between single isolated units or to visualize intramolecular energy migration. However, these EET processes take place on a timescale of a few picoseconds or even faster, which exceeds the temporal resolution of conventional SMS techniques. Here we present a new experimental approach to determine EET rates in a donor-acceptor-system on a single molecule level by influencing the photon statistic in a pump-pump like experiment. We excite the donor repetitively with a laser pulse train consisting of two pulses identical in terms of wavelength, polarization and power, separated by a variable time delay. After an excitation in the first pulse the donor moiety can only absorb a photon in the second pulse if it has decayed into the ground state by transferring its excitation energy to the acceptor. Using the technique of time correlated single photon counting (TCSPC) we can measure the probability for such a double excitation of our donor-acceptor system as a function of the time delay between the two pulses and therefore get access to the EET time constant.

CPP 63.4 Thu 10:15 C 264

Hyperbranched PAMAM/ Kaolinite Nanocomposites: Decoupling phenomenon and conductivity mechanism — •Shereen Omara[1,2], Gamal Turky[2], Mona H Abdel Rehim[2], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und- prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — [2]National Research Centre (NRC), 33 El Behouth St., Dokki, Giza, P.O.12622, Egypt

Increasing demands of the daily life requires a continuous discovering of new and tailored properties of materials that can be utilized in covering the requirements in several fields. Hyperbranched polymers (HBPs) are macromolecules that are characterized by a highly branched structure and multiplicity of reactive end groups, which could be promising for numerous applications. Here, hyperbranched poly(amidoamine) (HPAMAM)/ Ka nanocomposites was prepared via an in-situ polymerization and an ex-situ method. The latter approach leads to a partly intercalated structure of the nanocomposites, while the former method results in an exfoliated morphology. A combination of different techniques such as broadband dielectric spectroscopy (DBS), SXAS, FTIR, TEM, and DSC are employed to study the prepared samples. For the HPAMAM/ Ka-DCA nanocomposites (an ex-situ samples), the results indicated that the dc conductivity is increased by 4 orders of magnitude, with increasing concentration of the Ka-DCA. As an interesting result is that a significant decoupling between the characteristic time for conductivity relaxation and the segmental dynamics was observed, which depends on the concentration of the nanofiller.

CPP 63.5 Thu 10:30 C 264

Self-assembly of semiflexible polymers confined in thin spherical shells — •Mihir Khadilkar and Arash Nikoubashman — Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany

Confinement effects are critical for stiff macromolecules in biological cells, vesicles, and other confined systems. Here, the competition between the packing entropy and the enthalpic cost of bending is further shaped by strong confinement effects. Through coarse-grained molecular dynamics simulations of a semiflexible bead-spring model we discovered a rich phase behavior, including nematic ordering with an accumulation of chain ends in the equatorial plane as well as the emergence of bipolar and quadrupolar topological defects on the surface [1, 2]. To better understand the complex interplay between confinement and nematization, we investigate the self-assembly of semiflexible polymers confined in thin spherical shells as a function of chain length, packing density, chain stiffness, and shell thickness. We explore the range of ordered structures exhibited as the system changes from a monolayer to multiple layers, approaching bulk behavior. Relevant order parameters elucidate the nature of orientational ordering in different parameter regimes.
[1] Nikoubashman et al. Phys. Rev. Lett. 118, 217803 (2017)
[2] Milchev et al. J. Chem. Phys. 146, 194907 (2017)

CPP 63.6 Thu 10:45 C 264

Hierarchical excluded volume screening in solutions of bottlebrush polymers — •Jaroslaw Paturej[1,2] and Torsten Kreer[1] — [1]Leibniz Institute of Polymer Research Dresden, Germany — [2]University of Szczecin, Poland

Polymer bottlebrushes provide intriguing features being relevant both in nature and in synthetic systems. While their presence in the articular cartilage optimizes synovial joint lubrication, bottlebrushes offer pathways for fascinating applications, such as within super-soft elastomers or for drug delivery. However, the current theoretical understanding lacks completeness, primarily due to the complicated interplay of many length scales. During the talk analytical model will be presented demonstrating how structural properties of bottlebrushes depend on the concentration, ranging from dilute solutions to highly concentrated melts. The validity of our model is supported by data from extensive molecular dynamics simulations. We demonstrate that the hierarchical structure of bottlebrushes dictates a sequence of conformational changes as the solution concentration increases. The effect is mediated by screening of excluded volume interactions at subsequent structural parts of the bottlebrushes. Our findings provide important insights that should enable improved customization of novel materials based on the architectural design of polymer bottlebrushes.

15 min. break

CPP 63.7 Thu 11:15 C 264

Conformational relaxation of chains in highly entangled polymer melts after a large step deformation — •Hsiao-Ping Hsu and Kurt Kremer — Max Planck Institute for Polymer Research

Anisotropic stress relaxation of strongly deformed polymer melts in a non-linear viscoelastic regime and the resulting anisotropic structures of chains after isochoric elongation are studied. Both the classical Doi-Edwards tube theory and refined GLaMM tube theory incorporating contour length fluctuation, and convective constraint release predict that the process of retraction in entangled linear chains sets in immediately after the deformation, while there exist contradictions between experiment and theory. Our results of radius of gyration in the direction perpendicular to the stretching direction indicate chain retraction in the initial relaxation process. Applying the harmonic spherical expansion approach to the 2D scattering function along the parallel and perpendicular to the stretching direction, the profiles of the first anisotropic term of scattering function also qualitatively agree with the theoretical prediction by GLaMM around Rouse time. The influence of finite-size effects is also investigated. Finally, applying the primitive path analysis to the deformed polymer melts, we also observe that there exists significantly delayed equilibration processes while deformed polymer melts are relaxing.

CPP 63.8 Thu 11:30 C 264

Dissipation Controls the Relaxation Pathways of Collapse of a Polymer — •Suman Majumder, Henrik Christiansen, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

Variations in the nature of interactions with a solvent trigger various conformational transitions associated with macromolecules, e.g., the collapse of a polymer. Having this fact in hindsight, here, we investigate the kinetics of collapse of a model homopolymer in explicit solvent via a modified dissipative particle dynamics that allows qualitative tuning of the particle-velocity dissipation or in other words the solvent viscosity. As a generic phenomenon, the collapse follows a pathway characterized by the "pearl-necklace" picture (local clusters of monomers connected by strings of monomers) before eventually collapsing to a globule. However, as the viscosity increases, the time span of the "pearl-necklace" picture shortens and the dynamics appear to be dominated by de Gennes' "sausage-like" structures, which only in the long run approaches a compact spherical globule. We provide a novel way of separation of the time scales involving the "pearl-necklace" stage and the relaxation of the "sausage-like" structures based on cluster identification and shape factor analyses, respectively.

CPP 63.9 Thu 11:45 C 264

Relaxation of Disentangled and Collapsed Polymer chains in a melt — •Majesh Kumar Singh, Hsiao-Ping Hsu, and Kurt Kremer — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128, Mainz, Germany

Entanglements dominate the rheological behavior of high molecular weight polymeric melts. Experimental studies [1] show that slow and careful melting of disentangled polymer crystals lead to formation of metastable melt exhibiting lower viscosity. With an objective of studying the non-linear rheological behavior of fully disentangled globules in a melt under elongation, we follow the similar strategies developed in Ref. [2], and perform standard bead-spring model based molecular dynamics simulations to our polymer melt systems. The system is prepared by first forming independent single globules of polymer chains. We observe that for short chains ($N \leq 200$) our melt systems of disentangled globules reach their entangled and fully equilibrated state at $t \approx \tau_{R,N}$ ($\tau_{R,N}$: the Rouse time for chains of size N) while for $N = 1000$, the system has not reached its equilibrated state even at $t \approx 10\tau_R$. Through the primitive path analysis [3], we show the development of entanglements during the relaxation process from disentangled globules to entangled states. [1] Rastogi, et al. Nat. Mater. 4, 635 (2005). [2] Vettorel, Kremer, Macromol Theory Simul. 19, 44 (2010). [3] Everaers, et al. Science 303, 823 (2004).

CPP 63.10 Thu 12:00 C 264

Transitions between diblock copolymer lamellar orientations in shear flow — •Ludwig Schneider and Marcus Müller — University of Göttingen, Institute of Theoretical Physics, Göttingen, Germany

Shear alignment of microphase-separated materials is a well known strategy to manipulate self-assembled samples towards macroscopic anisotropy. However, details about the exact mechanism of the reorientation towards equilibrium states, previously trapped in meta-stable states, remain an open research question.

A constant shear flow is applied to a melt of symmetric diblock copolymers. The subsequent transition between the unstable (parallel) and the stable (perpendicular) lamellar configuration is investigated. The hypothesis for the transition of an unstable lamellar grain in a stable matrix is either i) the rotation of the grain in the matrix, ii) a growth and shrink process extinguishing the unstable grain, or iii) a melting of the unstable grain with a subsequent reorientation of the stable orientation.

Using Molecular Dynamics simulation, we observe two different mechanisms as a function of shear rate: At high shear rate, none of the hypotheses apply. Instead, we observe a fast transition where the unstable grain looses its orientation order and disintegrates into a microemulsion-like state with a characteristic length scale. We believe that this scenario is realized in LAOS experiments. At low shear rate, the slow transition proceeds via the shrinking mechanism iii).

CPP 63.11 Thu 12:15 C 264

Towards understanding three-body contributions to coarse-grained force fields — •Christoph Scherer and Denis Andrienko — MPIP, Mainz, Germany

CG is a systematic reduction of the number of degrees of freedom (DOF) used to describe a system of interest. CG can be thought of as a projection on the CG DOF and is therefore dependent on the number and type of CG basis functions. We present an extension of the two-body basis set with three-body basis functions of the Stillinger-Weber type with a flexible angular potential. The CG scheme is implemented in the VOTCA-CSG toolkit [1]. We show that naive extensions of the CG force-field can result in substantial changes of the two-body interactions making them much more attractive. This is related to the three-body basis functions having a significant two-body component which we examine in detail by decomposing the two-body potential of mean force (PMF). This interference can be alleviated by CG the two- and three-body forces separately which also helps to evaluate the importance of many-body interactions for a given system. The approach is illustrated on liquid water where three-body interactions are essential to reproduce the structural properties [2,3], and liquid methanol where two-body interactions are sufficient to reproduce the main features of the atomistic system. Our findings motivate to systematically extend the CG basis set in a way to clearly separate the many-body contributions of different order. [1] Rühle, Junghans, Lukyanov, Kremer, Andrienko, JCTC, 5, 3211 (2009); [2] Molinero, Moore, JPCB, 113, 4008 (2009); [3] Larini, Lu, Voth, JCP, 132, 164107 (2010)

CPP 63.12 Thu 12:30 C 264

Molecular Dynamics Simulation of Twin Polymerization via SDAT-ReaxFF — •Janett Prehl[1], Thomas Schönfelder[1], and Joachim Friedrich[2] — [1]Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany — [2]Institut für Chemie, Technische Universität Chemnitz, Chemnitz, Germany

Twin polymerization enables the formation of two different macromolecular structures from organic-inorganic hybrid materials in one single process step. To investigate in structure formation process on the atomic scale we utilize reactive molecular dynamics simulation via the SDAT-ReaxFF force field [1-3]. This recently developed extention of the ReaxFF force field is capable to cope with the complexity of the reaction mechanism of twin polymerization. The new feature of SDAT-ReaxFF is to define several atom types per chemical element instead of only one, as it is in the orginial ReaxFF.

In this presentation we introduce the SDAT-ReaxFF in the context of Twin Polymerization. We will show that we are able to model all partial reaction steps and the subsequent polymerization with this approach.

[1] T.Schönfelder et al., *Chem Phys* **440** (2014) 119–126

[2] J.Prehl et al., *J Chem Phys C* **121** (2017) 15984–15992

[3] K.H.Hoffmann, J.Prehl Reac Kinet Mech Cat DOI: 10.1007/s11144-017-1303-y

CPP 63.13 Thu 12:45 C 264

Cononsolvency of PNIPAM in Aqueous Methanol Solutions — •Cahit Dalgicdir[1], Francisco Rodríguez-Ropero[2], and Nico F. A. van der Vegt[1] — [1]Technische Universität Darmstadt, Darmstadt, Germany — [2]Illinois Institute of Technology, Chicago, United

States of America

A polymer might dissolve in the pure forms of two different solvents but may precipitate in mixtures of these solvents. This interesting phenomenon is called cononsolvency and poly(N-isopropylacrylamide) (PNIPAM) in aqueous methanol solutions is an example of it. Although cononsolvency for PNIPAM in water/methanol solutions is well known, the underlying mechanism and the driving forces are still under debate. Using extensive molecular dynamics simulations we find that the calorimetric enthalpy of the collapse transition shows a similar pattern compared to cononsolvency.[1] Polymer hydration is found to be the key factor for chain collapse where the hydrogen bonds between the water and the polymer amide are frustrated by methanol. [1]C.Dalgicdir, F.Rodríguez-Ropero, N.F.A. van der Vegt J. Phys. Chem. B, 2017, 121 (32)

CPP 64: Nanostructures, Nanostructuring and Nanosized Soft Matter II

Time: Thursday 9:30–12:45 Location: PC 203

CPP 64.1 Thu 9:30 PC 203

Spray deposition of conducting composite films studied with in situ GISAXS — •Volker Körstgens[1], Senlin Xia[1], Matthias Schwartzkopf[2], Calvin J. Brett[2,3], Daniel Söderberg[3], Stephan V. Roth[2,4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]DESY, 22607 Hamburg — [3]KTH, Fluidmechanics, SE-10044 Stockholm, Sweden — [4]KTH, Fibre and Polymer Technology, SE-10044 Stockholm, Sweden

In the emerging field of printable electronics there is a growing demand for transparent, flexible substrate materials. Cellulose-based substrates are a promising sustainable alternative to fully synthetic polymers. We present the fabrication of conducting composite films of cellulose nanofibrils (CNF) and PEDOT:PSS. CNF of high surface charge are produced with TEMPO (2,2,6,6-tetramethylpiperidine-1-oxyl radical)-mediated oxidation and mixed with PEDOT:PSS in aqueous dispersion. Composite films are produced with a spray deposition process which is followed in situ with GISAXS with subsecond time resolution. GIWAXS applied to the final films is used for the investigation of crystallinity in the composite films. Different CNF/PEDOT:PSS ratios and the influence of the additive glycerol on the film morphology and conductivity are investigated. The improvement of conductivity with the co-solvent glycerol and alternative post-treatment with ethylene glycol for the composite films follows the same trend as for pure PEDOT:PSS films.

CPP 64.2 Thu 9:45 PC 203

Homopolymer and Diblock Copolymer Blends with ABC Miktoarm Terpolymers — •Matthias M.L. Arras[1], Hyeyoung Kim[2], Monojoy Goswami[1], Hong Kunlun[1], Bobby G. Sumpter[1], Thomas P. Russell[2,3], and Gregory S. Smith[1] — [1]Oak Ridge National Lab, Oak Ridge, USA — [2]University of Massachusetts Amherst — [3]Lawrence Berkeley National Lab, Berkeley, USA

The effect of chain configuration in AB/ABC blends is investigated by small angle neutron scattering, transmission electron microscopy and molecular dynamics simulation. Here, the strongly segregating and asymmetric miktoarm star terpolymer poly(styrene)-*arm*-poly(isoprene)-*arm*-poly(2-vinylpyridine), where P2VP is the major component, was blended with equal volume fractions of either a PS/PI homopolymer mixture or an PS-*b*-PI diblock copolymer. We find that, depending on volume fraction, configuration and molar mass of the blended polymers, the morphology of the miktoarm star terpolymer is affected in various ways. In particular, swelling, improved ordering, or order-to-order transitions (OOT) were found. For low molar mass homopolymer blends (∼ 1/4 of the miktoarm block's mass) we find examples where the ordering of the blend has improved over the pristine miktoarm star. An OOT from a lamellar to hexagonal phase is induced by the diblock copolymer blend when its molar mass is similar to the one of the miktoarm blocks.

This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by ORNL. HK & TR were supported by AFOSR (16RT1602) and ARO (W911NF-17-1-0003).

CPP 64.3 Thu 10:00 PC 203

Effect of boehmite nanoparticles on mechanical properties and network architecture of epoxy — •Media Ghasem Zadeh Khorasani[1], Dorothee Silbernagl[1], Paulina Szymoniak[1], and Heinz Sturm[1,2] — [1]BAM, Berlin, Germany — [2]TU Berlin, Germany

Boehmite nanofillers (NP) were found to enhance mechanical properties of epoxy nanocomposites. Understanding the underlying mechanism requires investigations on structure-property relationship. Thus, we study the mechanical properties of anhydride-cured epoxy with boehmite NP (up to 15%wt) using AFM-based methods: force distance curves (FDC) and intermodulation AFM (ImAFM). FDC measurements show increase in stiffness of epoxy in the presence of boehmite but cannot resolve NPs. ImAFM stiffness maps with a resolution of ~10 nm reveal an unexpected increase in stiffness of epoxy matrix which implies structural change in the matrix. To investigate these changes dynamic mechanical analysis (DMA) is performed yielding viscoelastic properties and nanostructure of the cross-linked networks. We observe significant inhomogeneity and uncured residues in the neat epoxy which gradually disappear with increasing concentration of NP. In the case of 15wt% NP, despite of an increase in storage modulus of the glassy state, the rubbery state storage modulus and the crosslinking density decrease drastically. Based on these observations, we propose a new mechanism in which boehmite particles not only interact with epoxy matrix but also contribute to curing process and network structure.

CPP 64.4 Thu 10:15 PC 203

The influence of interfacial adhesion between a dispersed inorganic phase and a polymer matrix on the overall mechanical properties of composite materials — •Dorothee Silbernagl[1], Media Ghasem Zadeh Khorasani[1], and Heinz Sturm[1,2] — [1]BAM, Berlin, Germany — [2]TU Berlin, Berlin, Germany

The overall mechanical properties of composites are considered to correlate with the mechanical properties of the constituents, i.e. matrix phase (MP) and inorganic dispersed phase (DP). In the case of a MP, e.g. epoxy, which polymerizes in the presence of a DP, the mechanical properties of the interphase (IP), the organic matter in proximity to the filler particle, has to be taken into account. We show the major influence of a third parameter: the interfacial adhesion (IA) between MP and DP. In order to make this effect measurable a nanoparticle based composite was geometrically reduced to a substrate representing the DP and a thin polymer film (10 - 100 nm), representing the MP. Substrates with differently modified moieties enhancing or impeding the IA are used. Mechanical properties of such layered samples (silicon/PnBMA and boehmite/anhydride-cured epoxy) were measured by AFM force-distance curves (FDC), applying forces perpendicular to the interface. FDC curves show significant changes in deformation rates depending on the IA. This implies unexpected long range effect exceeding the effect of an IP.

CPP 64.5 Thu 10:30 PC 203

Self-Assembly of Discotic Rings and Nanowires in a Liquid Crystal Confined in Nanopores — •Kathrin Sentker[1], Arne Zantop[2], Arda Yildirim[3], Milena Lippmann[4], Tommy Hofmann[5], Oliver Seeck[4], Andriy Kityk[6], Andreas Schönhals[3], Marco Mazza[2], and Patrick Huber[1] — [1]Institut für Werkstoffphysik und -technologie, TU Hamburg — [2]MPI für Dynamik und Selbstorganisation — [3]BAM,Berlin — [4]DESY,Hamburg — [5]HZG für Materialien und Energie — [6]Faculty of Electrical Engineering, TU Czestochowa

Discotic Liquid Crystals (DLC) tend to stack up into linear columns creating charge carrier pathways along the stacking direction due to overlapping pi - electrons. Embedding DLCs into nanoporous membranes enables the preparation of organic molecular nanowires or nanorings. We show by high-resolution optical birefringence and synchrotron-based X-ray diffraction, as well as Monte Carlo simulations, that confining a thermotropic DLC in cylindrical silica nanopores induces a quantized formation of annular layers consisting of concentric circular bent columns, unknown in the bulk state [1]. Starting from the walls this ring self-assembly propagates layer-by-layer towards the pore center. In addition, we found a pore size dependent orientational transition from the circular to axial orientation in anodic aluminum oxide nanopores allowing the preparation of semiconductive organic nanowires. [1] Sentker et al., Quantized Self-Assembly of Discotic Rings in a Liquid Crystal Confined in Nanopores, 2017, submitted

CPP 64.6 Thu 10:45 PC 203

Unraveling the role of TTBC isomers in self-assembled tubular aggregates — •Jörg Megow[1], Tillmann Klamroth[1], Hans von Berlepsch[2], Craig N. Lincoln[3], and Jürgen Hauer[3] — [1]Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam — [2]Freie Universität Berlin, Fabeckstr. 34a, 14195 Berlin — [3]Technische Universität München, Lichtenbergstraße 4, 85748 Garching

In [1], a structure model for mono-walled tubular aggregates of 1,1',3,3'-tetraethyl-5,5',6,6'-tetrachloro-benzimidazolocarbocyanine iodide (TTBC) was proposed. There, the relative intensities and excitation energies of J- and H-bands could be explained satisfactorily. In [2], two isomers of the TTBC molecule have been discussed. In our present work we found a variety of TTBC isomers in the electronic ground state using density functional theory (DFT). Hence, the question arises which of those isomers is/are involved in the building of TTBC aggregates. Our molecular dynamics simulations together with the DFT results now give a strong hint that TTBC molecules within a tubular structure adopt nearly flat conformations which do not correspond to any of the geometries of the different ground state isomers. This can be explained by the rather flat potential energy surface of the TTBC conformational space.

[1] C. Friedl, T. Renger, H. v. Berlepsch, K. Ludwig, M. Schmidt am Busch, and J. Megow, Phys. Chem. C, 2016, 120 (34), 19416 [2] M. Aydin, Ö. Dede, and D.L. Akins, J. Chem. Phys., 2011, 134(6):064325

15 min. break

CPP 64.7 Thu 11:15 PC 203

Time resolved analysis of a Brownian motor — •Christian Schwemmer[1], Stefan Fringes[1,2], Urs Dürig[1,3], and Armin Knoll[1] — [1]IBM Research - Zurich, Switzerland — [2]Institute of Physical Chemistry, University of Zurich, Switzerland — [3]SwissLitho AG, Zurich, Switzerland

Artificial Brownian motors mimic the mechanism behind intracellular transport in nature [1] and enable a controlled transport of particles in a fluid [2]. In our implementation, we use a novel approach based on geometry induced trapping [3] to define a ratchet shaped potential landscape inside a nanofluidic slit. By applying a zero-mean AC electric field across the slit, we observed transport of 60 nm gold nano particles at drift speeds of 50 μm/s. The high temporal resolution of our experimental setup allowed us to measure the probability density *in-situ* and its temporal evolution with sub millisecond resolution. We observed current reversal at 250 Hz, an effect predicted more than 20 years ago [4], illustrating the nonlinear character of the motor. Comparison with a parameter-free theoretical model based on the Fokker-Planck equation shows excellent agreement. Using the model we traced the origin of the current reversal to the asymmetric, almost static probability density distribution at high frequencies, which leads to a faster increase of the backward current after switching the field direction.

[1] Vale et al., Science, **288**, 88, (2000)
[2] Hänggi et al., Rev. Mod. Phys, **81**, 387, (2009)
[3] Krishnan et al., Nature, **467**, 692, (2010)
[4] Bartussek et al., Europhysics Letters, **28**, 459, (1994)

CPP 64.8 Thu 11:30 PC 203

Interaction of Cationic Surfactants with Protein in Tubular Silica Nanopores Studied by Small-Angle Neutron Diffraction — Anja F. Hörmann[1], •Albert Prause[1], Viviana Cristiglio[2], Michael Gradzielski[1], and Gerhard H. Findenegg[1] — [1]Department of Chemistry, Technical University of Berlin, Berlin, Germany — [2]Institut Laue-Langevin, Grenoble, France

The interactions of surfactants with porous materials play an important role in environmental, chemical and medical applications. We studied nanostructures formed by adsorption and self-assembly of the cationic surfactants dodecyl pyridinium chloride (DPCl) and hexadecyl pyridinium chloride (CPCl) in the tubular mesopores of SBA-15 with pore diameter of 7 nm. Small-angle neutron diffraction (SAND) was used at silica contrast-matching conditions to obtain structural information from diffuse scattering contributions and the reappearance of the SBA-15 Bragg reflexes. For CPCl it could be shown that due to its high affinity to the negatively charged pore wall and the strong hydrophobic interaction of its tails the surfactant forms a monolayer *via* the growth of monolayer patches with increasing bulk concentration. Furthermore, we studied the co-adsorption of the globular protein lysozyme (Lyz) and CPCl. Whereas the pre-adsorption of CPCl is found to hinder the adsorption of Lyz sterically, the presence of Lyz seems to promote the homogeneity of the adsorbed material at the pore wall, as visible in the appearance of hollow cylinder scattering at lower adsorption fraction of surfactant f_s.

CPP 64.9 Thu 11:45 PC 203

Salt-induced microheterogeneities in binary liquid mixtures — •Markus Bier[1], Julian Mars[2], Hailong Li[2], and Markus Mezger[2] — [1]Max Planck Instutite Int. Sys. and University of Stuttgart, Germany — [2]Max Planck Institute Poly. Res. and University of Mainz, Germany

The formation of microheterogeneities (MHs) in binary liquid mixtures due to the presence of salt is investigated by means of small-angle X-ray scattering (SAXS) and liquid state theory. The phenomenon is experimentally known to occur for antagonistic salts, whose cations and anions prefer different components of the solvent mixture. However, up to now the origin of the characteristic length scale of MHs was unclear. In this contribution it is shown that MHs can be generated by an interplay between short-ranged interactions and long-ranged monopole-dipole interactions. This conclusion has been reached by performing SAXS measurements and comparing the solvent structure factor with a general expression derived without assuming any specific model. This method allows one to analyse the dependency of the MH structure with respect to ionic strength and temperature. Upon approaching the demixing phase transition, critical-like behaviour occurs close to the spinodal line in the phase diagram.

Reference:
M. Bier, J. Mars, H. Li & M. Mezger, Phys. Rev. E **96**, 022603 (2017).

CPP 64.10 Thu 12:00 PC 203

AC electrokinetic manipulation of nanoparticles and molecules — Eva-Maria Laux[1], Xenia Knigge[1], Christian Wenger[2], Frank F. Bier[1], and •Ralph Hölzel[1] — [1]Fraunhofer Institute for Cell Therapy and Immunology, Bioanalysis and Bioprocesses, Potsdam-Golm (IZI-BB), Germany — [2]IHP GmbH - Leibniz Institute for Innovative Microelectronics, Frankfurt (Oder), Germany

AC electric fields are increasingly exploited for the separation of nanoparticles and molecules in micro- and nanoelectrode systems. AC electrokinetic phenomena like dielectrophoresis (DEP) and AC electroosmosis allow a robust non-contact spatial manipulation. Here we present results of dielectrophoretic experiments on nanoparticles and proteins in various electrode systems. Numerous protein species have been successfully manipulated: intrinsically fluorescing proteins like eGFP, DsRed and RPE, and fluorescently labeled BSA; specific antibody binding as well as enzymatic function are shown to be retained after DEP immobilisation. Depending on electrode size, molecules and nano-particles are isolated as singles between planar triangular electrodes or on arrays comprising up to 500,000 conical electrodes. Using fluorescence polarisation microscopy, permanent dielectrophoretic immobilisation of eGFP molecules is demonstrated with parallel alignment of the proteins' main axis along the electric field, and the relative orientation of the molecule's fluorophor is determined.

CPP 64.11 Thu 12:15 PC 203

Efficient hydrogen evolution on triple point fermion semimetal MoP — •Guowei Li[1], Gudrun Auffermann[1], Jian Zhang[2], Xinliang Feng[2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187, Dresden, Germany — [2]Center for Advancing Electronics Dresden (cfaed), Department of Chemistry and Food Chemistry, Dresden University of Technology, 01062, Dresden, Germany

Materials in topological state result in many exotic properties such as large magnetoresistance, high conductivity, and an intrinsic Hall effect. However, their function in the field of chemistry has generally been overlooked and has attracted little attention. The observation of extremely high conductivity and Weyl nodes in MoP motivates us to design high performance electrocatalyst. Mo-P co-doped carbon layer@MoP was synthesized and exhibits outstanding electrocatalytic activity for the hydrogen evolution reaction (HER) with an overpotential of 49 mV at the current density of 10 mA/cm^2, and a Tafel slope of 54 mV per decade in alkaline media. All these make it one of the best non-noble metal hydrogen evolution electrocatalysts and even approaches to that of commercial Pt/C catalyst. The formation of P-C and Mo-C bonding in the interface and layers were able to shape the band structure more favoring for the electron accumulation and de-localization, resulting the high HER activity with a large exchange current density. The results here show a new way for the modification of carbon coating, which we can used for designing of high-performance HER electrocatalysts in both acid and alkaline media.

CPP 64.12 Thu 12:30 PC 203

13C isotope enriched graphitic material for operando NMR studies of processes in electrochemical cells — •Anastasia Vyalikh[1], Victor Koroteev[2], Wolfram Münchgesang[1], Lyubov' Bulusheva[2], Alexander Okotrub[2], and Dirk C. Meyer[1] — [1]TU Bergakademie Freiberg, Freiberg, Germany — [2]Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia

We provide a multi-scale characterization of a 13C-enriched fine-grained graphitic material and explore two different ways of its modification through a high-temperature high pressure annealing and a room-temperature chemical treatment. It has been found that such modifications result in structural and textural changes caused by carbon layer arrangement and carbon hybridization state, that can significantly affect the behavior in various applications, including batteries. We have shown that a high degree of 13C isotope enrichment, as well as good long-term performances in Li-ion batteries, and, in particular, an improved NMR spectral resolution in the bromine-treated sample provide the materials studied in the present work to be suitable candidates for 13C NMR study of processes in electrochemical cells.

CPP 65: Granular Matter / Contact Dynamics (joint session DY/CPP)

Time: Thursday 10:00–13:00 Location: BH-N 333

CPP 65.1 Thu 10:00 BH-N 333

Predicting contact numbers in granular packings — •Matthias Schröter[1], Simon Weis[2], and Gerd Schröder-Turk[3] — [1]Institute for Multiscale Simulation, University Erlangen, Nägelsbachstrasse 49b, 91052 Erlangen, Germany — [2]Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany — [3]School of Engineering and Information Technology, Murdoch University, 90 South Street, Murdoch, WA 6150, Australia

The mechanical stability of granular packings depends on the number of contacts its individual particles form with their neighbors. While these contact numbers can be measured using X-ray tomography [1], there are very few theoretical results prediciting this crucial parameter. A major part of the reason why theory lacks behind here is the frictional nature of the contacts [2]; up to now no effective method has been found to handle the inequality given by Coulomb friction. On the other side there is an abundance of experimental data. This raises the question if training an artificial neural network might be more effective to predict contact numbers than asking human experts.

[1] Schaller, Neudecker, Saadatfar, Delaney, Schröder-Turk, and Schröter, Physical Review Letters **114**, 158001 (2015)
[2] Schröter, EPJ Web of Conferences **140**, 01008 (2017)

CPP 65.2 Thu 10:15 BH-N 333

Rotator crystals in a granular monolayer — •Simeon Völkel and Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

The collective behaviour of vertically vibrated hexagonal disks confined in a horizontal monolayer is investigated experimentally. The disks tend to rotate upon sufficiently strong driving. Additionally, they can arrange in a hexagonal structure, reminiscent of a rotator crystal in equilibrium systems. We investigate the transitions into and out of this non-equilibrium steady state and their dependence on the presence of a wetting liquid. Furthermore we characterize the rotator crystal state using the bond orientational order parameter, parameters coupled with set voronoi diagrams, as well as the distribution of particle orientations. Finally we explore the influence of the disk's shape by varying the number of corners systematically.

CPP 65.3 Thu 10:30 BH-N 333

Collisional charging enhances aggregation in granular gases — •Chamkor Singh and Marco G. Mazza — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077, Goettingen, Germany

Since classical antiquity lightnings have been associated with the ashes produced during volcanic activity. It has been long speculated that collisional charging may play a significant role in particle's aggregation in such natural processes, *e.g.*, in the formation of planetesimals during the early stages of the birth of a planet, charging in dust devils, lightnings in thunderclouds, and electric sparks in dunes. We perform molecular dynamic simulations in three dimensions for a dilute, freely-cooling granular gas of viscoelastic particles that exchange charges during collisions. Using percolation theory, we find a stronger power law growth of the average cluster size, $S(t) \sim t^z$, with $z \approx \frac{3}{2}$ in the *collisionally charged* gas than $z \approx \frac{6}{5}$ in the *neutral* case. Remarkably, z is found to be independent of the typical Bjerrum length, or equivalently, of the ratio of characteristic Coulomb to thermal energy. However, this ratio alters the crossover time of the growth. The velocity distribution of the charged viscoelastic particles does not show a relaxation towards Maxwellian within the early stages of aggregation.

CPP 65.4 Thu 10:45 BH-N 333

Structural Evolution of Planar Granular Media — •Clara Wanjura[1], Takashi Matsushima[2], Othmar Marti[1], and Rafi Blumenfeld[3,4,5] — [1]Ulm University, Germany — [2]University of Tsukuba, Japan — [3]Inst. of Physics, Chinese Academy of Sciences, China — [4]Imperial College London, UK — [5]Cambridge University, UK

Granular materials are ubiquitous in nature, but continuum models of their macroscale behaviour and properties have proved to be difficult. Particle-scale properties and the structure affect strongly the large-scale behaviour.

Here we study a key characteristic of the structure in two dimensions: the cell-order distribution (COD). We first describe the evolution of the COD by a set of master equations and establish their validity by comparison to simulation data. The structure and the COD evolve mainly by contact making and breaking events. Of these, we identify and quantify 'non-clapping' events as the most relevant to the COD evolution and distinguish these from the less relevant 'clapping' events, which only add noise to the dynamics. The role of the cell order transition rates and their behaviour in the master equations are studied in detail analytically and numerically.

This formalism can be extended to the study of other structural characteristics.

CPP 65.5 Thu 11:00 BH-N 333

Optical Properties of Granular Matter — Dominik Kiese, Koray Önder, Sebastian Pitikaris, Matthias Sperl, and •Philip Born — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51147 Köln, Deutschland

Dense packings of hard spheres exhibit strong local ordering, even with lacking long-range order. The point pattern associated with the short-range order of hard sphere packings are shown to exhibit a photonic band-gap, i.e. a complete suppression of wave propagation for wavelengths similar to the center-to-center particle distance [1]. Common center-to-center distances in real granular media are millimetric, and suppression of THz waves reminiscent of development of a photonic bandgap have been observed [2]. We present an experimental study on the evolution of this bandgap with manipulating the structural order in granular packings. Local order in sedimented particle packings is controlled by mixing ratio and size ratio in binary packings. The relation among the bandgap and the structure offers a tool quickly quantify local order and to track structural changes in agitated granular media. We give an outline how to compute the band structure of hard-sphere packings taking into account the full spatial distribution of the dielectric constant.

[1]L. S. Froufe-Pérez et al., Physical Review Letters 117, 053902 (2016).

[2] P. Born. K. Holldack, Review of Scientific Instruments 88, 051802 (2017).

15 min. break

CPP 65.6 Thu 11:30 BH-N 333

Aeolian sand sorting and megaripple formation — Marc Lämmel[1], Anne Meiwald[1], Hezi Yizhaq[2], Haim Tsoar[3], Itzhak Katra[3], and •Klaus Kroy[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany — [2]Dpt. of Solar Energy and Environmental Physics, Blaustein Inst. for Desert Research, Ben-Gurion University of the Negev, Israel — [3]Dpt. of Geography and Environmental Development, Ben-Gurion University of the Negev, Israel

Sand is blown across beaches and deserts by turbulent winds. The seemingly chaotic process creates two dominant bedforms: decametre-scale dunes and centimetre-scale ripples, but hardly anything in between. By the very same process, grains are constantly sorted. Smaller grains advance faster, while heavier grains trail behind. Here, we argue that, under erosive conditions, sand sorting and structure formation can conspire to create distinct bedforms in the forbidden wavelength gap between aeolian ripples and dunes. These so-called megaripples are shown to co-evolve with an unusual, predominantly bimodal grain-size distribution. Combining theory and field measurements, we generate a mechanistic understanding of their shape and migration speed, as well as their cyclic aging, renewal, and sedimentary memory, in terms of the intermittent wind statistics. Our results demonstrate that megaripples exhibit close similarities to dunes and can indeed be mechanistically characterised as a special type of (“reptation”) dunes.

CPP 65.7 Thu 11:45 BH-N 333

Rheology of 3D frictionless spherocylinders — •Dániel B. Nagy[1], Tamás Börzsönyi[1], Philippe Claudin[2], and Ellák Somfai[1] — [1]Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Hungarian Academy of Sciences, Budapest, Hungary — [2]Physique et Mécanique des Milieux Hétérogènes, PMMH UMR 7636 ESPCI - CNRS - Univ. Paris-Diderot - Univ. P.M. Curie, Paris, France

The rheology of dense granular matter is an active domain of research and important both from the fundamental and the applied point of view. In the absence of large gradients, a successful approach formulates the constitutive equation as an effective friction μ, dependent only on the dimensionless inertial number I. In our work we used 3D numerical simulations to extend this formalism to frictionless spherocylinders. As in the case of spherical particles, the effective friction is an increasing function of the inertial number. We systematically investigated the dependence of μ on the particle aspect ratio Q, as well as that of the normal stress differences, the volume fraction and the coordination number. We found an interesting non-monotonic behavior of the quasistatic friction coefficient with Q: from the spherical case $Q = 1$, it first sharply increases, reaches a maximum around $Q \approx 1.05$, and then gently decreases until $Q = 3$, passing its initial value at $Q \approx 2$. We provided a microscopic interpretation for this through the analysis of the distribution of dissipative contacts around the particles. For slightly elongated grains the dissipation density is highest in their central cylindrical band, whereas at larger Q this moves to their caps.

CPP 65.8 Thu 12:00 BH-N 333

Controlling Segregation and Convection in Vibrofluidised Granular Media — •Christopher Windows-Yule[1,3], Anthony Rosato[2], and David Parker[3] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]New Jersey Institute of Technology, Newark, NJ, USA — [3]University of Birmingham, Edgbaston, Birmingham, UK

The convective and segregative behaviours of granular materials are of great relevance to myriad industrial and natural processes, yet - despite significant research - remain incompletely understood and infamously difficult to control. In this talk, we detail a series of combined experimental and simulational studies in which we elucidate a deep interrelation between these two important phenomena, and novel manners in which this interrelation may be exploited. In particular, we demonstrate manners in which careful manipulation of the geometry and excitation method of a vibrofluidised system may be used to augment, reduce, induce, suppress and otherwise control both convective and segregative phenomena.

CPP 65.9 Thu 12:15 BH-N 333

Rheology of Dense Granular Fluids: Theory & Experiment — •Till Kranz[1,2], Olfa Lopez[1], Annette Zippelius[3], Matthias Fuchs[4], and Matthias Sperl[1,2] — [1]Institut für Materialphysik im Weltraum, DLR Köln — [2]Institut für Theoretische Physik, Uni Köln — [3]Institut für Theoretische Physik, Uni Göttingen — [4]Theorie der Weichen Materie, Uni Konstanz

Granular fluids have been found to display a complicated rheology including Newtonian, shear thinning as well as shear thickening regimes. For a continuum description of granular flows, a constitutive equation is required that captures high densities and high shear rates.

We will introduce simple arguments regarding the time and energy scales in the system to explain the different flow behaviors. Newtonian rheology is expected at the lowest densities and shear rates only, shear thinning is related to the granular glass transition [1], and Bagnold scaling [2] is a consequence of hard-core interactions and shear heating. We will show how these constraints can be made quantitative in the framework of *Granular ITT* (Integration Through Transients) [3]. We will present experimental results for the flow behavior measured in a fluidized bed Couette cell that are well described by our theoretical approach.

[1] W. T. Kranz, M. Sperl and A. Zippelius, Phys. Rev. Lett. **104**, 225701 (2010)
[2] R. A. Bagnold, Proc. Royal Soc. A **225**, 49 (1954)
[3] W. T. Kranz, F. Frahsa, A. Zippelius, M. Fuchs and M. Sperl, arXiv:1710.04452, arXiv:1710.04475

CPP 65.10 Thu 12:30 BH-N 333

Simulation and modeling of the frustrated packing in a granular system — •Sára Lévay[1], David Fischer[2], Ralf Stannarius[2], Balázs Szabó[3], Tamás Börzsönyi[3], and János Török[1] — [1]Department of Theoretical Physics, BME, Budafoki út 8., H-1111 Budapest, Hungary — [2]Institute of Experimental Physics, Otto von Guericke University, Universitätsplatz 2., D-39106 Magdeburg, Germany — [3]Wigner Research Centre for Physics, Hungarian Academy of Sciences, P.O. Box 49., H-1525 Budapest, Hungary

Optimal packings of uniform spheres is a solved problem in two and three dimensions. The two-dimensional ground state can be easily achieved by simple dynamical processes while in three dimensions this is almost impossible.

In a recent work we have shown that in $2+\varepsilon$ dimensions, achieved by a container in one dimension slightly wider than the spheres, the particles organize themselves in a triangular lattice touching either of the sides of the container. When the system is agitated, it evolves slowly towards the potential energy minimum through metastable states.

We show results of DEM simulations and Monte Carlo models which fit the experiments: The dynamics is local and is driven by the optimization of the volumes of 7-particle configurations and by the vertical interaction between touching spheres. Defects in the triangular lattice play an important role in the dynamics as they act as an activation source and help the compaction. The system behaves neither as a 2D nor as a 3D system. Geometric frustration hinders the global optimum.

CPP 65.11 Thu 12:45 BH-N 333

Frustrated packing in a granular system confined in a $2+\varepsilon$ dimensional box — •David Fischer[1], Sára Lévay[2], János Török[2], and Ralf Stannarius[1] — [1]Institute of Experimental Physics, Otto von Guericke University, Universitätsplatz 2, D-39106 Magdeburg, Germany — [2]Department of Theoretical Physics, BME, Budafoki út 8., H-1111 Budapest, Hungary

Packing of spheres in three dimensions necessarily involves geometrical frustration. The locally optimal tetrahedral packing is not space-filling. In contrast, the close-packed equilateral triangular lattice optimizes the packing of disks in a two-dimensional plane both globally and locally.

We show experimentally that inside a container of a width only slightly wider than the diameter of the spheres, the particles organize themselves in a quasi-triangular lattice touching either the front or back wall of the container. Under appropriate agitation (harmonic vertical vibrations) the system can be driven remarkably close to its ground state. Nevertheless, perfect order is practically never reached.

We demonstrate that the system can be described by 13 local 7-particle configurations and that the volume occupied by those configurations plays a key role in the redistribution dynamics of the system. Our studies offer insights into both the influence of geometrical constraints on random granular packing and a descriptive example of frustrated ordering, comparable to order in antiferromagnetic Ising spin models.

CPP 66: Microswimmers II (joint session DY/CPP/BP)

Time: Thursday 10:00–13:15 Location: BH-N 243

CPP 66.1 Thu 10:00 BH-N 243

Dynamical density functional theory for swarms of active microscopic circle swimmers — Christian Hoell, Hartmut Löwen, and •Andreas M. Menzel — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

The study of self-propelled particles and active microswimmers is an intensely growing field. However, mostly straight-propelling objects are addressed. In contrast to that, typical real objects are imperfect and show persistently bent trajectories, as investigated in the present case.

Recently, we introduced a first dynamical density functional theory to describe swarms of straight swimming microswimmers suspended in a fluid [1]. The theory includes all basic ingredients, namely, self-propulsion, hydrodynamic as well as steric interactions between the swimmers, and confinement by external potentials. We have now extended this theory to statistically characterize the collective behavior of microscopic circle swimmers [2].

To illustrate the statistical consequences of circle swimming [2], we consider confinement by a spherical trap. While straight-swimming objects tend to push outward against the confining barriers and only by spontaneous symmetry breaking collectively move around the trap, circle swimmers show a deterministic tendency of rotating around the confinement. An increasing tendency of circle swimming leads to localization of the swimmer density in the center of the trap. We have investigated both pusher- and puller-type swimming mechanisms.

[1] A. M. Menzel et al., *J. Chem. Phys.* **144**, 024115 (2016).
[2] C. Hoell et al., *New J. Phys.* in press (2017).

CPP 66.2 Thu 10:15 BH-N 243

Memory-induced transition to persistent rotational motion for active colloids in viscoelastic media — •Narinder Narinder[1], Clemens Bechinger[1,2], and Juan Ruben Gomez-Solano[1] — [1] *2.Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany* — [2] *Max-Planck-Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany*

Life in nature is strongly conjoined with viscoelastic fluids, such as human blood and mucus. Thus, understanding the behavior of artificial microswimmers [1] in such fluids holds the potential for applications such as targeted drug delivery and cargo transport. Motivated by this, we study the dynamics of active colloids in a viscoelastic fluid. Investigating the fluid in the linear rheological response regime, with the increase in propulsion speed, a strong enhancement of the rotational diffusion of the particles is observed [2]. Further increase in the propulsion velocity of the particles leads to the emergence of a new behavior, in which particles describe well defined circular trajectories. Characterization of these orbits, reveals a non-linear dependence of the angular speed on the propulsion speed. We propose that these circular trajectories, absent in Newtonian fluids, originate from a persistent torque acting on the particles which stem from the strong coupling of particles directed motion to microstructural relaxation of the fluid.

[1] J. R. Gomez-Solano et al., Sci. Rep. 7, 14891 (2017).
[2] J. R. Gomez-Solano et al., Phys. Rev. Lett. 116, 138301 (2016).

CPP 66.3 Thu 10:30 BH-N 243

Mesoscale turbulence in active suspensions subjected to orienting external fields — •Henning Reinken[1], Sebastian Heidenreich[2], Markus Bär[2], and Sabine H. L. Klapp[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany — [2]Mathematische Modellierung und Datenanalyse, Physikalisch-Technische Bundesanstalt, Berlin, Germany

Active fluids show a variety of self-sustained non-equilibrium phenomena. An intriguing example is the emergence of a turbulent state in bacterial suspensions, denoted as mesoscale turbulence [1]. Recent publications have shown that a fourth order field theory for the collective microswimmer velocity describes the main features of mesoscale turbulence, including the emergence of a typical vortex size [2,3]. This theory couples the polar order parameter of the microswimmers to the solvent velocity and can be derived from a microscopic Langevin model including hydrodynamic and steric interactions via the Fokker-Planck equation [3,4]. In this work, we extend the theory towards the impact of orienting external fields (e.g. for magnetotactic bacteria or gravitactic algae cells). Using linear stability analysis and weakly nonlinear analysis, we investigate the influence of such external fields on the emerging structures. In addition, we verify our results via numerical solution of the equations.

[1] M. Marchetti et al., Rev. Mod. Phys. **85**, 1143 (2013).
[2] J. Dunkel et al., New J. Phys. **15**, 045016 (2013).
[3] S. Heidenreich et al., Phys. Rev. E **94**, 020601(R) (2016).
[4] H. Reinken et al., in preparation.

CPP 66.4 Thu 10:45 BH-N 243

Cluster formation of microswimmers with individually controlled motility — •Tobias Bäuerle[1], Andreas Fischer[2], Thomas Speck[2], and Clemens Bechinger[1] — [1]Universität Konstanz, Germany — [2]Johannes Gutenberg Universität Mainz, Germany

One of the most interesting aspects of microswimmers is their ability to form dynamical clusters even in the absence of long-ranged interactions. Previous experiments and simulations have demonstrated the occurrence of phase separation into large clusters and a dilute gas phase when the density and motility of the particles is sufficiently high. In contrast to previous studies, where the particle motility was kept constant in space and time, in our experiments we are able to control the motility of each single microswimmer depending on its surrounding, e.g. the local density and configuration of microswimmers. Using a light-activated system, such individual motility control is achieved by a feed-back system consisting of a rapidly scanned laser beam and a real-time particle detection algorithm. By introducing appropriate interaction-rules we demonstrate that formation of clusters can occur already at very small particle densities and that their shape and density can be modified by small variations in the interaction rules.

CPP 66.5 Thu 11:00 BH-N 243

Optimal decision making for sperm chemotaxis in the presence of noise — •Justus A. Kromer[1], Steffen Märcker[2], Steffen Lange[3], Christel Baier[2], and Benjamin M. Friedrich[3] — [1]Stanford University, Stanford CA, USA — [2]TU Dresden, Dresden, Germany — [3]cfaed/TU Dresden, Dresden, Germany

Navigating agents such as biological cells rely on noisy sensory input. In cells performing chemotaxis, such noise arises from the stochastic binding of signaling molecules at low concentrations. We theoretically address the classic problem of chemotaxis towards a single target. As application example, we study chemotaxis of marine sperm towards the egg. Recent experiments revealed that these cells are able to dynamically switch between slow and fast chemotactic steering. The benefit of this decision making remains open.

We reveal an inherent coupling between the speed of chemotactic steering and the strength of directional fluctuations that result from the amplification of noise in the chemical input signal. This implies a trade-off between slow, but reliable, and fast, but less reliable steering. By formulating optimal navigation in the presence of noise as a Markov decision process, we show that dynamic switching between slow and fast steering substantially increases the probability to find the egg. This decision making is most beneficial, if chemical signals are above detection threshold, yet signal-to-noise ratios of gradient measurements are low. This situation generically arises at intermediate distances from the egg, thus defining a 'noise zone' that cells have to cross.

15 min. break

CPP 66.6 Thu 11:30 BH-N 243

Crowd localisation and cohesion of micro-swimmers with perception-dependent motility — •Francois Lavergne, Hugo Wendehenne, and Clemens Bechinger — Department of Physics, University of Konstanz, 78464 Konstanz, Germany

The origin of crowd formation and cohesion in natural contexts remains an important question of collective dynamics, especially in the absence of taxis, communication, confinement, or attractive forces between the individuals. In this work, we show that the mere variation of the motility depending on the perception of other individuals is enough to induce such behaviour. We introduce a long-range indicator of crowd perception that only assumes the ability of an individual to count others within its vision cone. When this quantity exceeds a certain threshold for a given individual, its velocity is increased. This simple rule is applied in an experiment involving photo-responsive colloidal micro-swimmers, whose velocities can be individually varied by live-tuning the intensity of laser spots directed onto them. We observe that initially very dilute ensembles of these micro-swimmers localise into isolated groups, with virtually empty surroundings in unbound space, in sharp contrast with the long-time diffusive behaviour expected in the case of a constant motility. These groups remain cohesive, despite the activity of individuals within them and the absence of alignment, due to a kinetic stabilisation mechanism stemming from the modulation of the motility upon the non-reciprocal perception.

CPP 66.7 Thu 11:45 BH-N 243

Maximum in density heterogeneities of active swimmers — •Fabian Jan Schwarzendahl and Marco G. Mazza — Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

Suspensions of unicellular microswimmers such as flagellated bacteria or motile algae exhibit spontaneous density heterogeneities at large enough concentrations. Based on the relative location of the biological actuation appendages (i.e. flagella or cilia) microswimmers' propulsion mechanism can be classified into two categories: (i) pushers, like E. coli bacteria or spermatozoa, that generate thrust in their rear, push fluid away from them and propel themselves forward; (ii) pullers, like the microalgae Chlamydomonas reinhardtii, that have two flagella attached to their front, pull the fluid in and thereby generate thrust in their front. We introduce a novel model for biological microswimmers that creates the flow field of the corresponding microswimmers, and takes into account the shape anisotropy of the swimmer's body and stroke-averaged flagella. We characterize the nonequilibrium phase diagram, as the filling fraction and Péclet number are varied, and find density heterogeneities in the distribution of both pullers and pushers, due to hydrodynamic instabilities. We find a maximum degree of clustering at intermediate filling fractions and at large Péclet numbers resulting from a competition of hydrodynamic and steric interactions between the swimmers. We develop an analytical theory that supports these results. This maximum might represent an optimum for the microorganisms' colonization of their environment.

CPP 66.8 Thu 12:00 BH-N 243

Chemotactic interactions in systems of active and passive colloids — •Julian Stürmer[1], Dhruv Singh[2], Maximilian Seyrich[1], Peer Fischer[2], and Holger Stark[1] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]MPI-IS, Heisenbergstr. 3, 70569 Stuttgart, Germany

Self-propelled particles exhibit a variety of self-assembled dynamic structures. In particular, mixtures of active and passive colloids crystallize into 2D clusters as a result of chemotactic interactions [1]. The active colloids represent Janus particles that move while creating sinks in a chemical concentration field. The passive colloids react to the corresponding chemical gradients in form of a diffusiophoretic drift velocity towards the active particles. We model the mixtures using Langevin equations and a diffusion equation for the chemical field extending our approach in [2]. With increasing interaction strength, we observe a gaslike state, an oscillatory and finally a collapsed state. We study the clustering dynamics by quantifying the cluster growth and measuring the cluster velocity as a function of cluster size.

In a similar approach, we model a system of solely active colloids that interact via translational and rotational diffusiophoresis. Here, we take into account the asymmetric character of the Janus particles by including dipole contributions in the chemical concentration field. This asymmetry gives rise to interesting collective phenomena, e.g. the formation of chains that has been observed in recent experiments.

[1] D. P. Singh et al., Adv. Mater. 1701328 (2017)

[2] O. Pohl et al., Phys. Rev. Lett. 112, 238303 (2014)

CPP 66.9 Thu 12:15 BH-N 243

Modular microswimmers formed by ion-exchange particles — •Andreas Fischer, Ran Niu, Thomas Palberg, and Thomas Speck — Institut für Physik, Johannes-Gutenberg-Universität Mainz, Germany

Colloidal ion exchange particles generate solvent flow due to a combination of electroosmosis and electrophoresis, which induces long-range attractive interactions between the colloidal particles [1]. These interactions lead to the formation of colloidal "molecules" of varying size and structure. By breaking reciprocality, these molecules can be made active. Depending on their composition, we observe passively diffusing, linearly and circularly moving molecules with different propulsion velocities. We develop a model based on conservative interactions, which makes quantitative predictions about the swimmers' motion that we compare to the experimental results.

CPP 66.10 Thu 12:30 BH-N 243

The droplet divisome — Kyle A. Baldwin, Babak Vajdi Hokmabad, and •Corinna C. Maass — MPI für Dynamik und Selbstorganisation Göttingen

Active emulsions of nematic liquid crystals in micellar surfactant solutions are a flexible and well controlled model system for microswimmers, exhibiting a wealth of features like helical swimming, convection driven clustering, chemotaxis and autochemotaxis. Their propulsion is driven by Marangoni stresses caused by self-supporting instabilities in the interfacial surfactant coverage. Generally, such surface tension variations should deform the droplet interface, but we have not seen measurable deviations from a spherical shape for $50\mu m$ droplets in Hele-Shaw cells due to strong capillary forces. However, in experiments using squeezed droplets, i.e. larger, more disk-shaped objects in strong two-dimensional confinement, capillary forces are weakened due to an effective switch from areal to line tension and a decrease of the deformable interface to volume ratio. We have observed multipolar Marangoni instabilities, visible deformation during self propulsion and a spontaneous self division cascade for arrested droplets.

CPP 66.11 Thu 12:45 BH-N 243

Dynamical arrest in active emulsions — •Babak Vajdi Hokmabad and Corinna C. Maass — MPI für Dynamik und Selbstorganisation Göttingen

Liquid crystal (LC) droplets self-propel in an aqueous surfactant solution due to Marangoni flow at the droplet's interface. This propulsion is sustained by micellar solubilization of the LC phase. The solubilization leads to a secretion of filled surfactant micelles in the trail of the swimming droplet. This causes depletion of empty micelles in the trail and thereby trail avoidance. We have directly imaged the secretion and spreading of the filled micelles by adding fluorescent dye to the LC phase. The decay of the extracted Gaussian profiles in time is consistent with the theoretical diffusive spreading. Using this technique, we are able to visualize the chemotactic interaction of a swimmer with a trail. To study the collective dynamics of this autochemotaxis-dominated system we track individual swimmers in dense droplet ensembles in 2D and 3D. Results show that in a crowded system, a potential landscape is formed with local minima between the trails. We report on dynamical arrest of the swimmers in transient cages formed inside these local minima.

CPP 66.12 Thu 13:00 BH-N 243

Active Double Emulsions — •Kyle A. Baldwin, Babak Vajdi Hokmabad, and Corinna C. Maass — MPI für Dynamik und Selbstorganisation, Göttingen

Active emulsions – solutions containing self-propelling microscopic droplets – display a rich variety of solo and collective swimming behaviours, from self-avoiding helices to collective raft formation, which are strongly influenced by factors such as wall proximity, autochemotaxis, and liquid crystal (LC) structure. Here, we report on the formation and swimming behaviour of active water-oil-water (WOW) double-emulsions; swimming LC oil droplets which carry a secondary inner water droplet. We observe new periodically oscillating swimming modes, and find that shell stability is strongly influenced by nematicity, which inhibits coalescence of the aqueous phases. The utility of these double emulsion swimmers as cargo carriers, and the ability to release this cargo on-demand, makes this system an ideal mechanism for chemical delivery to localised, switchable reaction sites, with prospects for drug delivery.

CPP 67: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VI (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Thursday 10:30–12:45 Location: HL 001

CPP 67.1 Thu 10:30 HL 001

Core-level spectroscopy with the *GW* approximation — •Dorothea Golze and Patrick Rinke — Department of Applied Physics, Aalto University, Espoo, Finland

Inner-shell spectroscopy is an important tool to characterize molecules, liquids and adsorption processes at surfaces. We present a new, accurate method for computing X-ray photoelectron spectra based on the *GW* approximation that overcomes the limitations of density functional theory based approaches. Green's function theory in the *GW* approximation has become the method of choice for addition and removal energies of valence electrons in solids and is now increasingly being applied to molecules. However, *GW* core-level spectroscopy has thus far not received any attention. In most *GW* implementations, the self-energy is computed in the imaginary frequency domain followed by an analytic continuation to the real frequency axis. However, our calculations show that the analytic continuation becomes highly inaccurate for frequencies far away from the Fermi level and is not suitable for the computation of core excitations. Thus, we evaluate the self-energy on the real-frequency axis using the contour deformation (CD) technique. We implemented CD in combination with a resolution-of-the-identity approximation for the screened Coulomb interaction in the FHI-aims program package. Test calculations reveal that our implementation reproduces Turbomole reference calculations [1] perfectly. Furthermore, we present benchmark studies of small and medium-sized gas-phase molecules and discuss the potential of our method for more complex systems. [1] M. J. van Setten et al. JCTC, 2013, 232

CPP 67.2 Thu 10:45 HL 001

***GW* and beyond from matrix resolvents** — •Jan Gesenhues[1], Dmitrii Nabok[2], Michael Rohlfing[1], and Claudia Draxl[2] — [1]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [2]Theoretische Festkörperphysik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Typically GW calculations make use of either plasmon pole models or numerical integration in order to determine the screened Coulomb interaction W. We demonstrate how to obtain an analytical representation of W with the help of a matrix resolvent and present some standard GW results which have been obtained with the method. The analytical W is a useful starting point for subsequent calculations involving vertex corrections. On the other hand, the matrix resolvent technique itself can be applied upon a BSE-like equation of motion for the polarizability to include vertex corrections.

CPP 67.3 Thu 11:00 HL 001

Electron-Magnon Scattering in Elementary Ferromagnets from First Principles: Lifetime Broadening and Kinks — Mathias C. T. D. Müller, •Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We study the electron-magnon scattering in bulk Fe, Co, and Ni within the framework of many-body perturbation theory implemented in the full-potential linearized augmented-plane-wave method. Starting from the *GW* approximation we obtain a Bethe-Salpeter equation for the two-particle (electron-hole) Green function, where single-particle Stoner excitations and collective spin-wave excitations (magnons) are treated on the same footing. We employ the solution of the Bethe-Salpeter equation to construct a self-energy that describes the scattering of electrons and magnons. The resulting renormalized electronic band structures exhibit strong spin-dependent lifetime effects close to the Fermi energy, which are strongest in Fe. In the case of Co and Ni, the renormalization gives rise to kinks in the electronic band dispersion at low binding energies, which we attribute to electron scattering with spatially extended spin waves. Furthermore, we find a band anomaly at larger binding energies in iron, which results from a coupling of the quasihole with single-particle excitations that form a peak in the Stoner continuum. This band anomaly has, in fact, been observed in recent photoemission experiments at the same energy and momentum.

CPP 67.4 Thu 11:15 HL 001

Effects of the Tamm-Dancoff approximation on the optical spectra of organic molecules — •Tobias Lettmann and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

When calculating excited state properties of electronic systems within the many-body perturbation theory (MBPT), the Bethe-Salpeter equation (BSE) needs to be solved. This is often done within the so called Tamm-Dancoff approximation (TDA), neglecting the coupling of resonant and anti-resonant excitations.

It is generally accepted that the TDA is justified for large, extended systems e.g. bulk crystals. However it has been shown that the TDA may no longer hold for some organic semiconductors[1]. In this talk we discuss the effects of the TDA on the resulting optical spectra of organic molecules of different sizes and investigate for which cases the TDA may still be justified.

[1] B. Baumeier et al: *J Chem. Theory Comput.*, 2012, **8**, 997

CPP 67.5 Thu 11:30 HL 001

Ab-initio treatment of non-local electronic correlations with the dynamical vertex approximation — •Anna Galler[1], Patrik Thunström[2], Patrik Gunacker[3], Josef Kaufmann[3], Matthias Pickem[3], Jan M. Tomczak[3], and Karsten Held[3] — [1]Centre de Physique Theorique, Ecole Polytechnique, 91128 Palaiseau, France — [2]Department of Physics and Astronomy, Materials Theory, Uppsala University, 75120 Uppsala, Sweden — [3]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

Recently, approaches such as the dynamical vertex approximation (DΓA) or dual-fermion method have been developed. These diagrammatic approaches are going beyond dynamical mean-field theory (DMFT) by including non-local electronic correlations on all length scales as well as the local DMFT correlations. Here we present our efforts to extend the DΓA methodology to ab-initio materials calculations (AbinitioDΓA). Our approach is a unifying framework which includes both, GW and DMFT-type of diagrams, but also important non-local correlations beyond, e.g. non-local spin fluctuations. In our multi-band implementation we are using a worm sampling technique within continuous-time quantum Monte Carlo in the hybridization expansion to obtain the DMFT vertex, from which we construct the reducible vertex function in a ladder approximation. As a first application we show results for transition metal oxides. Support by the ERC project AbinitioDGA (306447) is acknowledged.

References: [1] A. Galler, P. Thunström, P. Gunacker, Jan M. Tomczak, and K. Held, Physical Review B 95, 115107 (2017)

CPP 67.6 Thu 11:45 HL 001

Non-local correlations in effectively reduced spatial dimensions — •Jan M. Tomczak[1], Matthias Pickem[1], Benjamin Klebel[1], Anna Galler[2], Josef Kaufmann[1], Patrik Gunacker[1], Patrik Thunström[3], Thomas Schäfer[2], Alessandro Toschi[1], and Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, Austria — [2]Centre de Physique Théorique, Ecole Polytechnique, Palaiseau, France — [3]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Using the dynamical vertex approximation and its recent extension for electronic structure calculations, AbinitioDΓA[1], we explore the impact of spatial dimensions onto non-local correlations: (a) we compare magnitude and manifestations of non-local self-energies in ultra-thin films of transition-metal oxides to those in the bulk material. (b) we track the evolution of non-local correlations in the doped Hubbard model when continuously going from 3D to 2D. In particular we probe the limits of the "space-time separation" of electronic correlations evidenced in 3D[2]. Support by the ERC project AbinitioDGA (306447) and the Austrian Science Fund (FWF) projects I 2794-N35 and P 30213-N36 is acknowledged.

References: [1] A. Galler, P. Thunström, P. Gunacker, JMT, K. Held, PRB 95, 115107 (2017), [2] T. Schäfer, A. Toschi, JMT, PRB 91, 121107R (2015)

CPP 67.7 Thu 12:00 HL 001

Does the optical signature of oxidized polyethylene stem from saturated or unsaturated carbonyl defects? — •Guido Roma[1], Fabien Bruneval[1], and Layla Martin-Samos[2] — [1]DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, F-91191 Gif sur Yvette, France — [2]CNR-Demokritos, Trieste, Italy

Polyethylene (PE), one of the simplest and most used aliphatic polymers, is generally provided with a number of additives, in particular antioxidants, because of its tendency to get oxidized. Carbonyl defects, a product of the oxidation of PE, are occurring in various forms, in particular saturated ones, known as ketones, where a C=O double bond substitutes a CH_2 group, and various unsaturated ones, i.e., with further missing hydrogens. Many experimental investigations of the optical properties in the visible/UV range mainly attribute the photoluminescence of PE to one specific kind of unsaturated carbonyls, following analogies to the emission spectra of similar small molecules. However, the reason why saturated carbonyls should not be optically detected is not clear. We investigated the optical properties of PE with and without carbonyl defects using perturbative GW and the Bethe-Salpeter equation in order to take into account excitonic effects. We discuss the calculated excitonic states in comparison with experimental absorption/emission energies and the stability of both saturated and unsaturated carbonyl defects. We conclude that the unsaturated defects are indeed the best candidate for the luminescence of oxidized PE, and the reason is mainly due to oscillator strengths.

CPP 67.8 Thu 12:15 HL 001

Bethe-Salpeter equation beyond the Tamm-Dancoff approximation at finite momentum transfer: Absorption and loss spectra including excitonic effects — •Benjamin Aurich, Caterina Cocchi, and Claudia Draxl — Humboldt-University, Berlin, Germany

The state-of-the-art ab-initio method for computing optical properties of semiconductors is based on the Bethe-Salpeter equation (BSE) which describes the excitations of the system in terms of interacting electron-hole (e-h) pairs. For absorption spectra, typically no momentum transfer from light to the e-h pairs is considered, and the coupling between excitations and de-excitations of e-h pairs is usually neglected by using the Tamm-Dancoff approximation (TDA). This approach yields excellent agreement with experiment for many materials, but may break down for confined systems [1]. The TDA is also known to fail to describe the electron energy loss spectra for materials as simple as silicon [2]. We report on the extensions of the open-source code `exciting` [3] allowing for BSE calculations beyond the TDA and at finite momentum transfer using an exact diagonalization scheme [4]. We demonstrate the differences between TDA and non-TDA spectra at vanishing and finite momentum transfer for periodic molecular systems.

[1] M. Grüning et al., Nano Lett **9**, 2820 (2009)
[2] V. Olevano and L. Reining, Phys. Rev. Lett. **86**, 5962 (2001)
[3] A. Gulans et al., J. Phys. Condens. Matter **26**, 363202 (2014)
[4] T. Sander et al., Phys. Rev. B **92**, 045209 (2015)

CPP 67.9 Thu 12:30 HL 001

Calculations of charge and spin susceptibilities and quasiparticle energy shifts within the CASTEP plane-wave DFT code — •Vincent Sacksteder[1], Evgeny Plekhanov[2], Phil Hasnip[3], Matt Probert[3], Stewart Clark[4], Keith Refson[1], and Cedric Weber[2] — [1]Royal Holloway University of London, UK — [2]Kings College London, UK — [3]University of York, UK — [4]University of Durham, UK

CASTEP is a pseudopotential based plane wave code which scales to the largest supercomputers and offers a wide feature set. Within CASTEP we have implemented calculation of the charge and spin susceptibility tensor, which describes the response to a perturbing charge or spin. We present corrections to the Kohn-Sham energies obtained by using the susceptibility tensor to screen Hartree-Fock exchange. In the static limit this is the SEX part of the COHSEX approximation, and if instead the dynamic susceptibility is used one obtains the GW approximation.

Our memory and CPU consumption scales linearly with the plane wave basis size, allowing thorough exploration of convergence with basis size, not only of the susceptibility itself, but of the SEX and GW quasiparticle shifts. We emphasize that our calculations are heavily parallelized, in exactly the same way as a standard DFT ground state calculation.

This work will allow first principles calculations of magnon spectra, exchange couplings, ionization potentials, and KKR and DMI coefficients.

CPP 68: Crystallization, Nucleation and Self-Assembly I

Time: Thursday 11:45–13:00 Location: C 230

CPP 68.1 Thu 11:45 C 230

Molecular self-assembly and dynamics on supramolecular polymers: impact of polarity and interactions strength — •Ana Bras[1], Marie Dorau[1], Daria Sokolova[1,2], Uxue Agirre[1,3], Ana Arizaga[1], and Annette Schmidt[1] — [1]Institute of Physical Chemistry, University of Cologne, Luxemburgerstr 116, Cologne (Germany) — [2]Chemistry Department, University of Basel, Basel (Switzerland) — [3]Faculty of Chemistry, University of the Basque Country, Donostia-San Sebastian (Spain)

The design of supramolecular polymers with novel or improved characteristics is an important segment on synthetic materials research. The present work focus on the self-assembly of low molecular weight polypropylene oxide (PPO) and polyethylene oxide (PEO) supramolecular polymers via H-bonding in the bulk. The pair diaminotriazine (Dat) and thymine-1-acetic acid (Thy), as well as 2-ureido-4[1H]-pyrimidinone (Upy) were the H-bonding groups of choice. Particularly SAXS and rheology were combined to study the correlation between the backbone polarity and the different groups interaction strength. Results on the structure show that PEO and PPO functionalized with Thy/Dat self-assemble as linear chains while functionalized with Upy show a sphere particle morphology corresponding to a Upy rich-phase, indicating phase separation. The corresponding Upy cluster radius is larger on PPO than on PEO due to the higher chain hydrophobicity. Moreover, the dynamical behavior indicates a dramatic change from predominantly viscous behavior as observed for Thy/Dat groups.

A.B. acknowledges DFG for a research grant (BR5303)

CPP 68.2 Thu 12:00 C 230

Structure Formation in Drying Colloidal Droplets — •Jiarul Midya and Arash Nikoubashman — Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany

The stratification dynamics of a polydisperse colloidal dispersion in a spherical droplet is investigated during its evaporation via molecular dynamics simulation. Here, our primary focus lies on the structure formation of the dispersed particles during the evaporation process. As the solvent evaporates, the particle concentration inside the droplet increases. Depending on the evaporation rate and the particle size ratios (characterized through the Peclet number), we observe the formation of a dense layer of smaller particles at the receding vapor-liquid interface, whereas the core of the droplet contains a mixture of both small and large particles. When the solvent is completely evaporated from the droplet a colloidal superparticle is formed, which can be porous, amorphous or crystalline, depending on material properties and evaporation rate.

CPP 68.3 Thu 12:15 C 230

Evaporation-induced assembly of colloidal crystals — •Michael P. Howard[1], Wesley F. Reinhart[1], Arash Nikoubashman[2], and Athanassios Z. Panagiotopoulos[1] — [1]Department of Chemical and Biological Engineering, Princeton University, Princeton, New Jersey, United States — [2]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany

Colloidal crystals have promising applications for technologies such as photonics, catalysis, and sensing. One convenient method to create such crystals is to disperse the colloids in solution and evaporate out the solvent, leaving behind a close-packed structure. In most situations, the crystal structures that form after evaporation are polycrystalline and highly sensitive to the processing conditions. For example, computer simulations have shown that in-plane crystalline order at the air-solvent interface undergoes a maximum with respect to evaporation rate. The influence of evaporation on crystal structure at larger scales, e.g, across multiple crystal layers, is not fully understood.

We performed massive-scale, explicit-solvent molecular dynamics simulations to study the evaporation-induced assembly of a colloidal crystal. We classified the structure of the crystallizing colloids using a machine-learning approach, and showed how the crystal nucleates and grows from the drying air-solvent interface. Complementary implicit-solvent simulations were performed to demonstrate the nontrivial role that solvent plays in controlling the crystallization process. Our work has important implications for the processing of colloidal crystals from solution and nonequilibrium molecular modeling.

CPP 68.4 Thu 12:30 C 230

Salt-induced temperature-dependent protein cluster formation: access to binding entropies and enthalpies — •Christian Beck[1,2], Marco Grimaldo[1], Michal Braun[2], Fajun Zhang[2], Felix Roosen-Runge[3], Frank Schreiber[2], and Tilo Seydel[1] — [1]Institut Laue Langevin, Grenoble, France — [2]IAP, University of Tübingen, Tübingen, Germany — [3]Physical Chemistry, Lund University, Lund, Sweden

With increasing Yttrium Chloride (YCl_3) salt concentration c_s, aqueous Bovine Serum Albumin (BSA) protein solutions subsequently change from a visually transparent (regime I) to a turbid phase (regime II) and back to a transparent phase (regime III: reentrant dissolution). Within regime II, a lower critical solution temperature (LCST) associated with a liquid-liquid phase separation (LLPS) can be observed. Quasi-elastic neutron scattering (QENS) data as a function of c_s and the protein concentration c_p lend support to the formation of protein clusters when approaching regime II [1]. By applying the Wertheim theory for patchy particles [2] and the Flory-Stockmeyer cluster size distribution function, it is possible to describe the temperature dependent cluster formation quantitatively. The ion-binding and protein-protein bridging entropies and enthalpies associated with the clusters can be determined directly from a simultaneous fit of the model to a large set of QENS spectra for different c_p, c_s, and T. The results are compared with calorimetry measurements [3]. [1]Grimaldo, M. *et al*, JPCL 6 (2015) 2577; [2]Wertheim, M., J. Stat. Phys. 1984, 35, 19-34; [3]Matsarskaia, O. *et al*, J. Phys. Chem. B 120 (2016) 7731

CPP 68.5 Thu 12:45 C 230

On the colloidal behavior of hybrid inorganic-organic lead halide perovskite precursor solutions and its impact on thin film microstructure — •Shambhavi Pratap, Johannes Schlipf, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Thin films based on crystalline hybrid organic-inorganic lead halide perovskites are processed by spincoating from precursor solutions of the organic and inorganic counterparts within suitably polar solvent systems (DMSO, DMF, GBL). The conditions of film formation follow non-equilibrium dynamics and resultant films display a range of microstructures including grain sizes, crystal strains, preferential orientations and remarkably, vivid hierarchical surface morphologies. By compositional engineering of the precursor, it is possible to tune the final film composition, as well as alter film morphology.

Colloidal nature of perovskite precursor solutions used for film fabrication is suggested, and phenomena such as glass-transitions, crystal twinning, and growth instabilities are explored in order to explain diffusion-limited self-organization of thin films. Microstructures are further demonstrated to be tunable by control of the colloidal chemistry of the precursor solution.

CPP 69: Focus: Polymers in Multi-Compartment and Aqueous Solutions I - organized by Jens-Uwe Sommer and Debasish Mukheri

Time: Thursday 15:00–18:30 Location: C 130

Topical Talk CPP 69.1 Thu 15:00 C 130

Biomimetic functions of hydrophobic-hydrophilic random copolymers — •Monica Olvera de la Cruz[1], Trung Nguyen[1], Baofu Qiao[1], and Ting Xu[2] — [1]Northwestern University, Evanston, IL, USA — [2]University of California, Berkeley, CA, USA

Random copolymers with hydrophobic and hydrophilic groups are multicomponent systems with important functionalities for biomimetic applications. They can dissolve in organic solvents and in water and as such can be used to disperse and stabilize enzymes in unfavorable solvents. In this talk, we address the key factors that govern the ability of random copolymers to adsorb to biological substrates including proteins. Our findings show that for sufficiently strong solvent selectivity there exists an optimal value of the copolymer adsorbing fraction that maximizes the surface coverage. The existence of the optimal adsorbing fraction is shown to result from the balance between the entropic and energetic gains accompanying the adsorption process. Full atom and coarse-grained simulations show that there is a clear connection between substrate surface composition and fraction of copolymer adsorbed, and that the adsorption is highly sequence selective by the substrate composition. The results in this work set the stage for computational design of random copolymers for stabilizing and delivering enzimes across multiple media.

CPP 69.2 Thu 15:30 C 130

Precision Polymer Engineering through Biomolecular Templates — •David Ng, Sean Harvey, Yu Tokura, and Tanja Weil — Max Planck Institute for Polymer Research, Mainz, Germany

Nature provides a host of macromolecules that are both specific in their functions as well as sequence. The absolute atomic positioning in three dimensional space provides a precision scaffold unrivalled in the synthetic world even in the years to come. It is therefore intuitive that by combining the vast spectrum of knowledge on protein and DNA architectures with polymer chemistry, a new platform that allows the customization of nanoscale features can be evolved.

In the first part, we will discuss the conceptual design of using the protein structure as a backbone to position polymers. Depending on the chemistry and the strategy, materials ranging from anisotropic hybrid nanostructures to stimulus responsive hydrogels can be constructed. In the second part, DNA origami technology is used to provide true programmable features. Persistent shapes that do not exist in nature can be first templated by the origami by which polymers can be designated and grown in limitless possibilities in a three dimensional space. Collectively, we show that the incorporation of bioarchitectures into nanotechnology is multifold, with implications that impact the design as well as further application of such systems.

CPP 69.3 Thu 15:45 C 130

Entropic Segregation in Mixtures of Dendrimers and Linear Polymer Solutions — •Martin Wengenmayr[1,2], Ron Dockhorn[1,2], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden, Germany

In mixtures of chemically compatible branched and linear polymers demixing effects are observed suggesting entropic forces caused by a difference in architecture only. For a better understanding of topological effects in mixtures of chemically identical polymers we investigate dendrimers of different sizes dissolved in a polymer solution of various chain lengths. We find that linear chains do always interpenetrate the volume of the dendrimer, whereas a collapsed state of the dendrimer known for poor solvent conditions, does not appear. Based on a scaling analysis of the dendrimer size we suggest that a thread length of the dendrimer, i.e. the longest path from the core to the terminal groups, is the relevant variable which should be compared with the chain length of the linear polymers. We can identify two scaling regions: When the chains are short compared to the length of the thread the dendrimer displays good solvent behavior, whereas longer chains lead to a θ-state of the dendrimer. Using umbrella sampling we observe an effective attraction between two dendrimers immersed in the solution of long linear chains. These insights are used to understand dendrimers used as processing aids in extrusion processes.

CPP 69.4 Thu 16:00 C 130

Orthogonally and doubly switchable diblock copolymers: Schizophrenic behavior — Natalya S. Vishnevetskaya[1], Viet Hildebrand[2], Bart-Jan Niebuur[1], Peter Müller-Buschbaum[1], André Laschewsky[2,3], and •Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Universität Potsdam, Institut für Chemie, Germany — [3]Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm, Germany

Doubly switchable diblock copolymers from blocks featuring lower and upper critical solution temperature behavior (LCST, UCST) may serve for advanced delivery purposes. We present results from diblock copolymers having a thermoresponsive LCST block and a zwitterionic UCST polysulfobetaine block, which is sensitive to ionic strength as well [1]. In aqueous solution, these diblock copolymers are expected to form core-shell micelles with the UCST block in the core and the LCST block in the shell or vice versa, i.e. so-called schizophrenic behavior. Depending on the values of the respective cloud points, the switching between these states may proceed via a molecularly dissolved state or via precipitation.

Using turbidimetry and small-angle neutron scattering, we investigate the phase behavior and the micellar structures in dependence on the choice of the two blocks and the block copolymer composition. Orthogonal and double switching behavior is identified and is found to depend crucially on these factors [1].

1. N. S. Vishnevetskaya et al., *Macromolecules* **49**, 6655 (2016) and **50**, 3985 (2017).

CPP 69.5 Thu 16:15 C 130

Kinetics of Mesoglobule Formation in Dependence on Pressure of Aqueous Poly(N-isopropylacrylamide) Solutions — •Bart-Jan Niebuur[1], Leonardo Chiappisi[2], Xiaohan Zhang[1], Florian Jung[1], Vitaliy Pipich[3], Marie-Sousai Appavou[3], Alfons Schulte[4], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Institut Laue-Langevin, Grenoble, France — [3]JCNS at MLZ, FZ Jülich, Garching, Germany — [4]University of Central Florida, Department of Physics, Orlando, U.S.A.

Aqueous solutions of the thermoresponsive polymer Poly(N-isopropylacrylamide) form stable mesoglobules above their cloud point. Their size and degree of hydration depend strongly on pressure [1]. To elucidate the early stages of mesoglobule growth, time-resolved small-angle neutron scattering is applied during pressure jumps which induce phase separation. In this way, the phase-separated state is reached extremely fast within few ms. At low pressure, two different growth processes are observed. The early stage of aggregation is diffusion-limited, followed by the appearance of an energy barrier, hindering the growth during later stages. The time at which the energy barrier starts to dominate depends strongly on the target pressure of the jump. At high pressure, only one growth process is observed, and the energy barrier hindering the aggregation is much smaller than at low pressure. Thus, the growth behavior seems to be closely related to the hydration state of the polymeric chains [1].

[1] B.-J. Niebuur et al., ACS Macro Lett. 6, 1180 (2017)

15 min. break

Topical Talk CPP 69.6 Thu 16:45 C 130

Soft matters in one-phase mixed solvents — •Takeaki Araki — Department of Physics, Kyoto University, Kyoto, Japan

We numerically study charged polymers and colloids in solvent mixtures. Even when the solvent is mixed in the bulk, local concentration inhomogeneities cause the attractive interactions among the solutes. (1) The behaviors of polyelectrolyte chains in solvent mixtures are investigated, taking into account the concentration inhomogeneity and the ionization. When changing the interaction parameters between the solvent components, we found a first-order transition of the polymer conformation. In the mixing state far from the coexistence curve, the polymers behave as semi-flexible chains. In the phase-separated state, on the other hand, they show compact conformations included in the droplets. As the interaction parameters of the mixture are increased, an inhomogeneous concentration field develops around the polymer and induces critical Casimir attractive interactions among the monomers. The competition between the electrostatic interactions and the critical Casimir ones gives rise to drastic changes in the conformation.(2) We studied the behavior of colloidal suspensions in solvent mixtures under shear flows. Far from the phase-separation point, they are well dispersed and the suspension exhibits a Newtonian viscosity. When the mixture is close to the coexistence curve, the particles aggregate by attractive interactions due to the concentration inhomogeneity, and the viscosity of the suspension increases.

CPP 69.7 Thu 17:15 C 130

Drunken polymers: How does a polymer swell in poor solvent mixtures? — •Debashish Mukherji[1], Carlos Marques[2], Torsten Stuehn[1], and Kurt Kremer[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128, Mainz, Germany — [2]Institut Charles Sadron, Universite de Strasbourg, CNRS, 23 rue du Loess, 67034, Strasbourg Cedex 2, France

Macromolecular solubility in solvent mixtures often strikes as a paradoxical phenomenon [1]. In a standard poor solvent, chains can collapse due to increased monomer-solvent repulsion interactions that lead to an effective attraction between monomer units, also known as depletion induced attraction. While polymer collapse in poor solvent is well understood, polymer swelling at intermediate mixing ratios of two repulsive solvents still lacks a microscopic explanation. Here we combine computer simulations and theoretical arguments to unveil the microscopic, generic origin of this collapse-swelling-collapse scenario. We show that this phenomenon naturally emerges at constant pressure in mixtures of purely repulsive components when a delicate balance of the entropically driven depletion interactions is achieved [2].

[1] D. Mukherji, C. M. Marques, and K. Kremer, Nature Communications 5, 4882 (2014). [2] D. Mukherji, C. M. Marques, T. Stuehn, and K. Kremer, Nature Communications 8, 1374 (2017).

CPP 69.8 Thu 17:30 C 130

Polymer brush in competitive solvents — •Andre Galuschko and Jens-Uwe Sommer — Leibniz-Institut für Polymerforschung Dresden e. V. Germany

By means of molecular dynamics simulation we study the equilibrium properties of a single polymer brush layer immersed in two good solvents (solvent and cosolvent), which induces for a single chain a coil-globule-coil transition depending on the co-/solvent-composition[1,2], called cononsolvency effect.

We extend the proposed simulation model in Ref.[2] to a homopolymer brush, where the solvent is treated implicitly and the cosolvent particles are simulated explicitly to mimic the concentration dependent composition. The attraction of cosolvent towards the monomer and the influence of grafting density are varied.

The recently developed theoretical description of an adsorption-attraction model for such scenario (Ref.[3]) is tested with our simulation results. We find very good agreement of our data and the proposed theory.

Additionally, we observe coexisting partially collapsed and swollen brush phases, which is coupled to a concentration-dependent Flory-Huggins mixing parameter as discussed in Ref.[3,4].

[1] Mukherji, Marques, Kremer, Nat. Commun. 2014, 5 ,p. 4882
[2] Heyda, Muzdalo, Dzubiella, Macromolecules 2013, 46, p. 1231
[3] Sommer, Macromolecules, 2017, 50, p. 2219
[4] Baulin, Zhulina, Halperin, J. Chem. Phys. 2003, 119, p. 10977

CPP 69.9 Thu 17:45 C 130

Lubrication by vapor-hydrated polymer brushes — Jan-Willem Nijkamp, Luuk van der Velden, Ilse de Vries, Jurjen Regenspurg, Sinem Tas, Hubert Gojzewski, Kristianne Tempelman, Nieck Benes, Julius Vancso, and •Sissi de Beer — University of Twente, Enschede, the Netherlands

Hydrophilic polymer brushes are well-know to be excellent lubricants when they are fully immersed in water. However, many applications require low-friction in air. We evaluate the water-distribution in hydrophilic polymer brushes in humid air and study the lubricating performance of these brushes as a function of the relative humidity using both molecular dynamics simulations and atomic force microscopy experiments. Our results show two characteristic maxima in the friction as a function of humidity, which indicates that there are multiple dynamic relaxations in the brush.

CPP 69.10 Thu 18:00 C 130

How robust is atomistic modeling of LCST of polyNIPAM? — Vladimir Palivec, Denis Zadrazil, and •Jan Heyda — University of Chemistry and Technology, Prague, Czech Republic

Poly-N-isopropyl acrylamide (PNIPAM) serves as a role model of thermoresponsive polymers in vast majority of computational studies. Our community relies, almost exclusively, on the OPLS-AA parameterization of PNIPAM, which was found promising in the early publication of Vrabec et al. (DOI: 10.1016/j.fluid.2010.03.025). Despite its usage over almost a decade, our knowledge comes only from independent long simulation runs at set of temperatures. An important warning was raised by a recent work of Kang et al. (DOI: 10.1021/acs.jpcb.6b09165), where microsecond swollen-collapse-swollen transition times were reported even for chain as short as 30mer. Notably, there is no simulation study in which equilibrium thermodynamics and LCST of the PNIPAM model are determined. In this contribution, we invest 1 milion CPU hours to shed light on this missing gap, and critically compare transition thermodynamics of available PNIPAM models.

CPP 69.11 Thu 18:15 C 130

Detailed calorimetric study on the collapse of poly(N-isopropylacrylamide) in aqueous sodium and guanidinium salts solutions — •Daniel Ondo, Adam Kovalčík, Jakub Polák, Vladimír Palivec, and Jan Heyda — University of Chemistry and Technology, Prague, Czech Republic

Poly(N-isopropylacrylamide) (pNIPAM) is a thermoresponsive polymer with a lower critical solution temperature (LCST) in pure water at 33 C. Addition of electrolytes, protein denaturants or organic cosolvents as a third component into aqueous pNIPAM mixtures, may change its solvation and balance between a collapsed hydrophobic and a swollen hydrophilic states hence alter the LCST and related thermodynamic quantities. In this work, employing the isothermal titration (ITC) and differential scanning (DSC) calorimetry, the LCST and total enthalpy of the collapse process of pNIPAM as a function of polymer and salt concentration (NaCl, Na_2SO_4, $NaClO_4$, NaSCN, GndCl, Gnd_2SO_4, GndSCN) were measured. Any effort to fit the calorimetric data by mass-action chemical binding or kinetic models failed. Nevertheless, the solvation of the collapsed polymer at 35 C is well described by Schellman's solvation model. The experimentally observed trends in LCST and total collapse transition enthalpy are in agreement with literature, verify the salt-polymer solvation model and are consistent with specifically designed dialysis measurements. Moreover, the microscopic details derived from the calorimetric measurements are in accord with performed μ-long atomistic simulations in the explicit solvent.

CPP 70: Crystallization, Nucleation and Self-Assembly II

Time: Thursday 15:00–18:15 Location: C 230

Invited Talk CPP 70.1 Thu 15:00 C 230

Crystallization in melts of semi-flexible hard polymer chains: An interplay of entropies and dimensions — •Wolfgang Paul and Timur Shakirov — Institut für Physik, Martin Luther Universität, 06099 Halle

Morphology selection upon crystallization of long-chain polymers is governed by an intricate and so far unresolved interplay between thermodynamic and kinetic effects. We argue, that the thermodynamic driving forces for this phase transition can be studied looking at relatively short chains as well. For a melt of short, semi-flexible polymer chains with purely repulsive intermolecular interactions, Stochastic Approximation Monte Carlo simulations can be employed to obtain the complete thermodynamic equilibrium information. Thermodynamics is obtained based on the density of states of a simple coarse-grained model, which varies by up to 5500 orders of magnitude. We show that our polymer melt undergoes a first-order crystallization transition upon increasing the chain stiffness at fixed density. The lyotropic three-dimensional orientational ordering transition drives the crystallization and is accompanied by a two-dimensional hexagonal ordering transition in the plane perpendicular to the chains. While the three-dimensional ordering can be understood in terms of Onsager theory, the two-dimensional transition is similar to the liquid-hexatic transition of hard disks. Due to the domination of lateral two-dimensional translational entropy over the one-dimensional translational entropy connected with columnar displacements, the chains form a lamellar phase.

CPP 70.2 Thu 15:30 C 230

Free energy barriers for crystal nucleation from fluid phases — •Peter Koss[1,2], Antonia Statt[3], Peter Virnau[1,2], and Kurt Binder[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 9, 55128 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [3]Princeton University, Princeton, NJ 08544, USA

A fluid in equilibrium, confined in a finite volume, with a density exceeding the onset of freezing, may exhibit phase coexistence with a crystal nucleus surrounded by liquid or a gas. Classical nucleation theory predicts that the barrier of homogeneous nucleation is comprised of two contributions, the free energy gained by the creation of a crystal droplet and the free energy loss due to surface tension of the newly created interface. We obtain the excess free energy due to the surface of the crystalline nucleus by using a computational method suitable for the estimation of the chemical potential of dense fluids. Our analysis method is appropriate for crystal nuclei of all shapes, without suffering from ambiguities occurring when one needs a microscopic identification of the crystalline droplet. We present an analysis method to determine the coexistence pressure between fluid and crystal, and the nucleation barrier for a soft version of the effective Asakura-Oosawa model at $\eta_p^r = 0.1$, 0.2 and 0.28 [1].

[1] P. Koß, A. Statt, P. Virnau, and K. Binder, Phys. Rev. E 96, 042609 (2017)

CPP 70.3 Thu 15:45 C 230

Additive modified crystallization in binary Lennard Jones system — •Bhaskar Sen Gupta, Marc Radu, and Kurt Kremer — Max Planck Instutute for Polymer Research, Mainz, Germany

Additive modified crystallization is ubiquitous in nature, e.g., during the growth of calcitic stalactites, of mollusk shells or of bone structures. Control of crystallization by additives has applications in many areas of science and technology, such as production of pharmaceuticals, semiconductors, and nonlinear optics, as well as formation of biominerals. We employ computer simulation to study the additive enhanced crystal growth in a binary Lennard Jones mixture under different scenarios. The crystal growth rate, the structure of the liquid solid interface and the interface morphologies strongly depend on the miscibility of the components. An accelerated crystal growth is observed for systems of poor solubility. We find the growth of different types of crystals and the growth dynamics depend on the structure of the interface which is determined by the solubility of the (non-crystalizing) minority component. It is also observed that the crystal growth mechanism follows the predictions of the Kardar-Parisi-Zhang theory in 2 + 1 dimensions for well miscible Lennard Jones mixtures.

CPP 70.4 Thu 16:00 C 230

Nucleation work in the crystallization of hard spheres — •David Richard and Thomas Speck — Staudingerweg 9, 55128, Mainz, Germany

Calculating the nucleation work associated with the spontaneous formation of a nucleus from a mother phase is not an easy task. On one side, classical nucleation theory (CNT) provides an accurate framework to compute the nucleation barrier associated with two coexisting bulk phases. On the other side, it fails to describe small nuclei composed of few hundreds (or even thousand) of particles. In this study, we combine a new approach to compute free energy barriers from brute force simulations and forward flux sampling without having to sample the dissolution of the nucleus. This method is applied to study the crystallization of hard spheres. We combine results from these simulations with seeding and equilibrium droplets [1,2], and make use of the nucleation theorem to evaluate the nucleation work for a large range of supersaturations. We present a direct comparison of this method with the capillary approximation present in CNT.

[1] Seeding approach to crystal nucleation. J. R. Espinosa, C. Vega, C. Valeriani, and E. Sanz, JCP (2016). [2] Finite-size effects on liquid-solid phase coexistence and the estimation of crystal nucleation barriers. A. Statt, P. Virnau, and K. Binder, PRL (2015).

CPP 70.5 Thu 16:15 C 230

Short-polyethylene systems: On the low-temperature states of single chains and few chain aggregates — •Timur Shakirov and Wolfgang Paul — Institute of Physics, University of Halle,

Halle, Germany

The phase behavior of polyethylene has been under investigation during many decades. But investigation of single-chain crystallization is a technically difficult problem. One of the reasons for this is that in the case of molecular dynamics simulations as well as in experiments, it is not so easy to distinguish thermodynamic and kinetic effects on chain folding. We here present results of a Wang-Landau type Monte Carlo simulation, which give a possibility to analyze thermodynamic equilibrium properties of a system. Our simulation study of short polyethylene chains is based on a chemically realistic united atom model [1]. Simulation results for deep-energy (or equivalently low temperature) states of single chains of different lengths demonstrate a set of various ground-state configurations: from stretched and hairpin-like configurations of short chains to a helix-like structure reeled round one of the chain's ends. Aggregates of a few chains demonstrate more complex behavior having disordered and ordered phases even for aggregates composed of a couple of chains. Corresponding low-energy configurations differ form configurations of single chains having the same length. However, with increasing chain length, single chain and aggregate morphologies become more similar.

[1] W. Paul, D. Y. Yoon, and G. D. Smith, J. Chem. Phys. 103 (1995) 1702-1709.

15 min. break

CPP 70.6 Thu 16:45 C 230

Polymorphism of syndiotactic polystyrene crystals studied by coarse-grained and atomistic simulations — •Chan Liu[1], Christine Peter[2], Kurt Kremer[1], and Tristan Bereau[1] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]Theoretical Chemistry, University of Konstanz, Konstanz, Germany

Syndiotactic polystyrene (sPS) has attracted both academic and industrial attention because of its complex polymorphic behavior upon crystallization. However, computational modeling of polymer crystallization is a challenging task because these processes are slow on the molecular time scale. From a combination of Coarse-grained (CG) modeling and Replica Exchange Molecular Dynamics (REMD), we study for the first time polymorphism of polymer crystals from simulations. In our work, we show that the CG model is capable to reproduce sPS crystallization at a transition temperature in good agreement with atomistic simulations. Main (alpha and beta) polymorphs found in annealing experiments occur in both atomistic and CG simulations. The CG model allows us to efficiently characterize polymorphism at a large scale.

CPP 70.7 Thu 17:00 C 230

In situ Formation and Growth Characterization of Iron Oxide Nanoparticles by Synchrotron X-Ray Scattering Techniques — •Robert Wendt[1,2], Eike Gericke[1,2], Anna Lang[2], Dragomir Tatchev[3], Giorgia Greco[1], Markus Wollgarten[4], Armin Hoell[1], Klaus Rademann[2], and Simone Raoux[1,5] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Institute for Nanospectroscopy, DE — [2]Humboldt-Universität zu Berlin, Department of Chemistry, DE — [3]Bulgarian Academy of Sciences, Institute of Physical Chemistry, Sofia, BG — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, Department of Nanoscale Structures and Microscopic Analysis, DE — [5]Humboldt-Universität zu Berlin, Department of Physics, DE

This work includes an innovative measurement setup for microwave-assisted nanoparticle syntheses which facilitates in situ investigations of pressurized colloidal solutions by allowing exact addition of precursor solution into the sealed vessel reactor and withdrawal of colloid solution at any time. Thereby, we are able to investigate and characterize the early stages from molecule to nanoparticle in a time-range of milliseconds by coupling in situ UV-Vis spectroscopy, synchrotron based Wide-Angle and Small-Angle X-ray Scattering. These in situ studies are combined with complementary ex situ methods, Transmission Electron Microscopy, Electron Energy Loss Spectroscopy and X-ray Absorption Spectroscopy. By combining these results, we provide concepts for formation and growth mechanisms of iron oxide nanoparticles which were synthesized by microwave-assisted solvothermal routes.

CPP 70.8 Thu 17:15 C 230

Tracking the reaction and film formation dynamics during in situ polymerization of polythiophene thin films — •Jenny Lebert[1], Eva Maria Kratzer[1], Stephan Pröller[1], Oliver Filonik[1], Philippe Fontaine[2], and Eva M. Herzig[3] — [1]TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany — [2]Synchrotron SOLEIL, 91192 Saint Aubin, France — [3]Universität Bayreuth, Physikalisches Institut, Herzig Group - Dynamik und Strukturbildung, 95440 Bayreuth, Germany

Native polythiophene belongs to the class of conjugated, semiconducting polymers which become conductive upon doping and therefore offer a broad range of potential applications in organic electronics. While polythiophene itself is insoluble, it is possible to obtain solution-processed thin films by employing an in situ polymerization technique.

Here, we present an experimental approach of tracking both, the reaction kinetics and film formation dynamics at the same time during the film formation employing simultaneous time-resolved UV/Vis transmission spectroscopy and grazing incidence wide angle X-ray scattering (GIWAXS). With this approach, we are able to characterize the intrinsic film formation phases. This allows us to suggest which processing parameters should be adapted in order to further improve the final film characteristics.

CPP 70.9 Thu 17:30 C 230

Biomolecule-Linked Plasmonic Nanoclusters as Colloidal SERS Sensors — •Roland Paul Maximilian Höller[1], Izabella Jahn[2], Dana Cialla-May[2], Jürgen Popp[2], Munish Chanana[3], Christian Kuttner[1,4], and Andreas Fery[1,4] — [1]Leibniz Institute of Polymer Research, 01069 Dresden, Germany — [2]Leibniz Institute of Photonic Technology, 07745 Jena, Germany — [3]Institute of Building Materials, ETH Zürich, 8093 Zürich, Switzerland — [4]Cluster of Excellence Centre for Advancing Electronics Dresden and Technische Universität Dresden, 01062 Dresden, Germany

We present controlled three-dimensional nanoassemblies with core/satellite architecture as colloidally stable probes for surface-enhanced Raman scattering (SERS). Aiming at obtaining a versatile system for bioapplications with both high and robust SERS performance, we used BSA as biomolecular linker for the controlled fabrication of self-assembled nanoclusters with correlated optical and structural properties by design [1]. The SERS performance of the assembled nanoclusters was benchmarked using an aromatic low-molecular-weight model analyte (4MBA). The characteristic signals of adsorbed 4MBA were detected with high robustness. The limit of detection of 10-6 M 4MBA was determined using non-enhanced volume-Raman signals of the medium as reference [2]. For bioapplication of such nanoassemblies, the aspects of biocompatibility, cellular uptake, and biological are decisive for a rational material design.

[1] R. P. M. Höller et al., ACS Nano, 2016, 10, 5740. [2] R. P. M. Höller et al., manuscript in preparation.

CPP 70.10 Thu 17:45 C 230

Temperature-dependent IR-transition moment orientational analysis applied to thin supported films of poly-ϵ-caprolactone — •Wilhelm Kossack[1], Martha Schulz[2], Thomas Thurn-Albrecht[2], Jörg Reinmuth[1], Viktor Skokow[1], and Friedrich Kremer[1] — [1]Molecular Physics department, Peter Debye Institut für weiche Materie, University Leipzig, Linnéstraße 5, 04103 Leipzig — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, FG Experimentelle Polymerphysik, 06120 Halle/Saale, Germany

Based on temperature dependent orientational infrared spectroscopy (Infrared Transition Moment Orientational Analysis), the three dimensional molecular order parameter tensors of IR-active transition dipole moments with respect to the sample coordinate system are determined during melting of Poly-ϵ-caprolcatone. Crystallinity and macroscopic order remain largely unaltered up to $T \sim 50°C$, above which they decline. This decrease reflects the melting of flat on crystalline lamellae, contributing about 34% to the crystalline material. The remaining crystallites are arranged as in two-dimensionally confined bulk-like spherulites, which melt by less than $(3\pm3)\%$. Consequently, flat on oriented lamellae are regarded kinetically favoured during confined melt crystallization, but thermo-dynamically less stable than spherulites.

CPP 70.11 Thu 18:00 C 230

Polymer self-assembly into nanoparticles through rapid solvent exchange in organic media — •Tatiana Morozova[1], Victoria E. Lee[2], Athanassios Z. Panagiotopoulos[2], Robert K. Prudhomme[2], Rodney D. Priestley[2], and Arash Nikoubashman[1] — [1]JGU, Mainz, Germany — [2]Princeton University, Princeton, USA

Polymeric nanoparticles (NP) are vital components for a wide range of applications, such as biomedical targeting and diagnostics. Recently, a new method to form monodisperse polymeric NPs was developed, which relies on the rapid micromixing of a polymer solution with a nonsolvent . Using this technique, stable NPs from hydrophobic polymer were fabricated in water without additional stabilizers. It was hypothesized that this peculiar stability might originate from electrostatic stabilization, mediated by the adsorption of hydroxide ions on the hydrophobic surface, water charge transfer effect, or possible impurities in the system. In order to elucidate the nature of the stabilization mechanism in the NP suspension, we conducted experiments using alternative organic nonsolvents instead of water, i.e. heptane and hexane. To our surprise, the polymers aggregated into stable NPs for a wide range of process parameters. We theoretically investigated possible explanations for this stability: steric, electrostatic stabilizations and conditional thermodynamic equilibrium. Our considerations suggest that electrostatic stabilization is the most likely candidate, but the source of the charge is still elusive as there are no obvious charge carriers in the system.

CPP 71: Organic Electronics and Photovoltaics - OLEDs and Molecular Excitations

Time: Thursday 15:00–18:00 Location: C 243

CPP 71.1 Thu 15:00 C 243

Intra- and Intermolecular TADF emission investigated by magnetic resonance methods — •Nikolai Bunzmann[1], Benjamin Krugmann[1], Sebastian Weissenseel[1], Gintare Grybauskaite-Kaminskiene[2], Dmytro Volyniuk[2], Andreas Sperlich[1], Juozas V. Grazulevicius[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg — [2]Kaunas University of Technology, Lithuania — [3]Bavarian Center for Applied Energy Research (ZAE Bayern)

Organic light emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF) utilize molecules with a small energy splitting ΔE_{ST} between singlet and triplet states. This can either be realized in intramolecular charge transfer states of molecules with near-orthogonal donor and acceptor moities or in exiplex states formed between a proper combination of individual donor and acceptor materials. Here, we investigate 4,4'-(9H,9'H-[3,3'-bicarbazole]-9,9'-diyl)bis(3-(trifluoromethyl) benzonitrile) (pCN-BCzmCF3), which shows intramolecular TADF but simultaneously can form intermolecular exciplex states in combination with 4,4',4"-Tris[phenyl(m-tolyl)amino]triphenylamine (m-MTDATA). In order to reveal which triplet states are involved in the RISC mechanism for both types of TADF emission, we apply electroluminescence and photoluminescence detected magnetic resonance (ELDMR, PLDMR). Thereby, we draw a comprehensive picture of which intermediate states are populated between optical or electrical excitation and light emission.

CPP 71.2 Thu 15:15 C 243

The interplay of TADF and phosphorescence in warm-white hybrid OLEDs — •Ludwig Popp[1], Paul Kleine[1], Ramunas Lygaitis[2], Reinhard Scholz[1], Simone Lenk[1], and Sebastian Reineke[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, TU Dresden, Germany — [2]Kaunas University of Technology, Lithuania

White emission in OLEDs is usually a combination of two or more different emitters with individual colors. Therefore, it is necessary that all included systems are efficient. It has been shown that the concept of thermally activated delayed fluorescence (TADF) allows to synthesize very efficient light-emitting molecules with various emission colors.

In our work, we use the sky-blue TADF emitter $5\mathrm{CzCF_3Ph}$ with an emission maximum at a wavelength of 495 nm, reaching a photoluminescence quantum yield of 70 % and up to 18% external quantum efficiency (EQE) in OLEDs. By combination with the common phosphorescent red emitter $\mathrm{Ir(MDQ)_2(acac)}$ within one emission layer it is possible to build warm white OLEDs with a high color rendering index of over 80 and correlated color temperatures about 2800 K.

Due to the variety of local and charge-transfer excited states in the emitter system, there are several probable scenarios for the energy transfer between $5\mathrm{CzCF_3Ph}$ and $\mathrm{Ir(MDQ)_2(acac)}$ since excitons are formed mostly on the TADF emitter. Utilizing time-correlated single photon counting (TCSPC) with a wavelength-sensitive detection, we deliver a thorough investigation of the exciton transfer and exchange mechanisms in the emitter system of our warm-white hybrid OLEDs.

CPP 71.3 Thu 15:30 C 243

Blue emitting TADF Materials for Organic Light Emitting Diodes — •Sebastian Weissenseel[1], Felix Klingert[1], Nikolai Bunzmann[1], Liudmila G. Kudriashova[1], Nikita Drigo[2], Mohammad Khaja Nazeeruddin[2], Andreas Sperlich[1], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Group for Molecular Engineering of Functional Materials, EPFL, CH-1951 Sion, Switzerland

Since the mechanism of thermally activated delayed fluorescence (TADF) emission was proposed for organic light emitting diodes (OLEDs), the OLED community experienced renewed enthusiasm. The molecular design of TADF materials omits the expensive heavy metal atoms needed for phosphorescence emitters and thus promises a cost reduction and sustainability. Here, we investigate novel blue emitting molecules, which exhibit intramolecular TADF mechanism. OLED devices are analyzed by means of current-electroluminescence-voltage characteristics, emission spectra and external quantum efficiency. We also apply direct spin-sensitive measurements on OLED devices to extract information about the involved spin states and shed some light on the TADF mechanism [1]. This may contribute to an overall better understanding of TADF, which is essential for further improvement of organic light emitting diodes.

[1] S. Vaeth, et al., Adv. Optical Mater. **5**, 1600926 (2017).

CPP 71.4 Thu 15:45 C 243

The Role of Molecular Environment in Thermally Activated Delayed Fluorescence — •Liudmila G. Kudriashova[1], Nikita Drigo[2], Sebastian Weissenseel[1], Andreas Sperlich[1], Mohammad Khaja Nazeeruddin[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg, Germany — [2]Group for Molecular Engineering of Functional Materials, EPFL, CH-1951 Sion, Switzerland — [3]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg, Germany

Thermally activated delayed fluorescence (TADF) opened the way to overcome the efficiency-limiting spin statistics in a new generation of organic light-emitting diodes (OLEDs). Intensity of intramolecular TADF is mainly ruled by conformation of the donor/acceptor parts within the emitter molecule and temperature. At the same time, the role of host matrix is poorly discussed in literature. Here, we report luminescent properties of novel TADF molecules studied in a broad range of temperatures in various types of solid films. We show that emission consists of three components: prompt fluorescence, delayed fluorescence and phosphorescence. Temperature and environment of the TADF emitters have crucial effect on lifetimes and relative amplitudes of the components. Hindering of the emitting molecules in a polymeric matrix suppresses phosphorescence, while increasing both TADF lifetime and intensity a hundredfold. All in all, we demonstrate that the molecular environment can significantly improve TADF efficiency, which is decisive for the resulting OLED performance.

CPP 71.5 Thu 16:00 C 243

Thermal spin polarization of OLEDs observed by correlated fluorescence and phosphorescence in dual emitters — •Tobias Scharff, Jonas Zipfel, Wolfram Ratzke, Sebastian Bange, and John M. Lupton — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Universitätsstraße 31, 93053 Regensburg, Germany

In organic light emitting diodes (OLEDs), injected charge carriers can undergo thermal relaxation processes. At low temperatures and high magnetic fields, where the Zeeman energy is comparable with the thermal energy, spin polarization can have a remarkable impact on the spin statistics of the electron-hole recombination process, which is monitored directly by electroluminescence. Here, we sensitize an organic semiconductor with a metal-free phenazine derivative which exhibits simultaneous fluorescence and phosphorescence. This approach allows us to study the impact of spin polarization on spin statistics directly through the ratio of fluorescence and phosphorescence, i.e. in an all-optical manner. Thermal spin polarization leads to an increase in phosphorescence with a concomitant decrease in fluorescence. Besides providing insight into carrier thermalization processes, the approach also offers a route to probing the effect of spin-orbit coupling on spin statistics.

CPP 71.6 Thu 16:15 C 243

Influencing and quantifying the intersystem crossing in biluminescent organic molecules by adding heavy atoms — •Felix Fries[1], Anna Haft[1], Ramunas Lygaitis[2], Olaf Zeika[1], and Sebastian Reineke[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials, TU Dresden, Nöthnitzer Str. 61, 01187 Dresden — [2]Kaunas University of Technology, K. Donelaičio g. 73, 44249 Kaunas

Organic molecules are able to show a broad variety of emission types. Fluorescence, phosphorescence or charge transfer (CT) state emissions have very different properties in energy and time regime. For one emitter, CT does not play a role and normally, those systems only show either fluorescence or phosphorescence. We name systems showing both fluorescence and phosphorescence at room temperature, biluminescent. An advantage of having experimentally access to both emission channels is that a very detailed description of the energetic behaviour of those molecules is possible. Here, we focus on a series of molecules with different levels of bromination. Namely those molecules are, N,N,N',N'-tetraphenyl-[1,1'-biphenyl]-4,4'-diamine (TPB) and Br$_x$TPB, where $x = 1 \ldots 4$. Extensive analysis of those molecules gives the luminescent lifetimes (∼ns, ∼ms), their contribution to the quantum yield and allows to quantify the intersystem crossing rate as a function of the bromination. Furthermore, the experimental results can be compared to numerical simulations like a line shape analysis of the radiative transitions, allowing deeper understanding of the influences of the heavy atom effect on the molecules' energetic landscape.

15 min. break

CPP 71.7 Thu 16:45 C 243

Photoswitchable Sn-Cyt c Solid-State Devices — Satoshi Nakamaru[2], William Ford[1], Yoshio Goto[2], and •Florian von Wrochem[1] — [1]Sony Europe Ltd., Materials Science Laboratory, Hedelfinger Strasse 61, D-70327 Stuttgart, Germany — [2]Advanced Materials Laboratories, Sony Corporation, Atsugi Technology Center No.2, 4-16-1 Okata, Atsugi, Kanagawa, 243-0021, Japan

Electron transfer across proteins plays an important role in many biological processes, including those relevant for the conversion of solar photons to chemical energy. Previous studies demonstrated the generation of photocurrents upon light irradiation in a number of photoactive proteins, such as photosystem I or bacteriorhodopsin. Here, we show that Sn-cyt c layers act as reversible and highly efficient photoelectrochemical switches upon integration into large area solid state junctions. Photocurrents are observed both in the Soret-band (lambda = 405 nm) and in the Q-band (lambda = 535 nm), with current on/off ratios reaching values of up to 25. The underlying modulation in charge transfer rate is attributed to a hole-transport channel, created by the photoexcitation of the Sn-porphyrin.

CPP 71.8 Thu 17:00 C 243

Conical intersection dynamics mediating coherent ultrafast singlet fission — •Hong-Guang Duan[1,2,3], Ajay Jha[1], Vandana Tiwari[1], Pabitra Nayak[4], Zheng Li[1], Michael Thorwart[2,3], and R. J. Dwayne Miller[1,3,5] — [1]MPSD, Hamburg, Germany — [2]I. Institut für Theoretische Physik, UH, Germany — [3]CUI, Hamburg, Germany — [4]University of Oxford, UK — [5]University of Toronto, Canada

Carrier multiplication in organic semiconductors by singlet fission holds the key to break the Shockley-Queisser limit. Primary step of singlet fission process is a spin-allowed transition of a singlet exciton to a doubly excited pair of spin-correlated triplets. Consequently, two triplets are formed after the spin decoherence. Despite enormous studies, the mechanism of the primary step is still unclear. Here, we use transient grating spectroscopy to probe the vibrational dynamics of singlet fission process in pentacene thin films. Our observations guide us to propose the existence of the conical intersection mediating singlet state and spin-correlated triplet pair transition. The interplay of vibrational modes mediating this transition will be discussed.

CPP 71.9 Thu 17:15 C 243

Excited States Dynamics in TIPS-Pentacene Studied with Femtosecond Time-Resolved Second Harmonic Generation — •Vipilan Sivanesan[1], Silke Koser[2], Uwe Bunz[2], and Petra Tegeder[1] — [1]Universität Heidelberg, Physikalisch-Chemisches Institut — [2]Universität Heidelberg, Organisch-Chemisches Institut

Understanding the ultrafast excited state dynamics in organic semiconductors after optical excitation is a key requisite on the road towards the design of efficient organic solar cells (OPV). Recently, the singlet fission process has gained much attention since it may improve the energy conversion efficiency in OPVs. In this work we monitored the ultrafast (sub-picosecond) excited states dynamics in TIPS-Pentacene (TIPS-Pn) using time-resolved second harmonic generation (TR-SHG). Sapphire was used as non-interacting substrate to analyse the dynamics of excitonic species in TIPS-Pn films. Thereby the dynamics of singlet fission process could be resolved. The process consists of the generation of singlet excitons localized on a single molecule followed by the fission into two triplet excitons on two TIPS-Pn molecules. While the overall singlet fission process occurred within 200fs, we could also resolve the transfer from the singlet exciton state to the mediating multiexciton state.

CPP 71.10 Thu 17:30 C 243

Direct observation of double hydrogen transfer via quantum tunneling in a single porphycene molecule on Ag(110) — •Matthias Koch[1], Mark Pagan[2], Mats Persson[2], Sylwester Gawinkowski[3], Jacek Waluk[3,4], and Takashi Kumagai[1] — [1]Fritz-Haber-Institut — [2]University of Liverpool — [3]Polish Academy of Sciences — [4]Cardinal Stefan Wyszyński University

Quantum tunneling of hydrogen atoms plays a crucial role in many chemical and biological reactions. Although tunneling of a single particle has been studied extensively in one-dimensional potentials, many-particle tunneling in high-dimensional potential energy surface remains poorly understood. Recently tautomerization of a single molecules was observed in LT-STM experiments [1, 2]. Here we present a direct observation of double hydrogen atom transfer within a single porphycene molecule on Ag(110) using a low temperature STM [3]. We find that below ~10 K the tautomerization rate is temperature-independent and a large kinetic isotope effect (KIE) was observed upon substituting the hydrogen atoms by deuterium. Inelastic electron tunneling increases the tautomerization rate by a vibrational excitation. The observed KIE for three isotopologues and density functional theory calculations indicate that a stepwise transfer mechanism is dominant in the tautomerization. This is also in agreement with the observed third state in our time dependent tip height traces.

[1] L. J. Lauhon et al. Phys. Rev. Lett. 85, 4566 (2000)
[2] T. Kumagai et al. Phys. Rev. Lett. 100, 166101 (2008)
[3] M. Koch et al. J. Am. Chem. Soc. 139 (36), 12681 (2017)

CPP 71.11 Thu 17:45 C 243

Nonlinear optical response of chromophores from real-time time-dependent DFT — •Caterina Cocchi[1], Stefano Pittalis[2], and Carlo A. Rozzi[2] — [1]Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — [2]CNR Istituto Nanoscienze, Modena, Italy

The impulsive excitation scheme for time propagation in time-dependent density-functional theory [1] can be efficiently adopted to study the optical response also beyond the linear regime, mimicking a broadband laser beam illuminating the sample. We demonstrate the potential of this approach by investigating the nonlinear optical response of carbon-conjugated chromophores, e.g., phthalocyanines and thiophenes, that absorb visible light of specific frequencies while being transparent to others. At increasing intensity of the applied field, the sharp peak giving the absorption edge in the linear regime loses weight, while the oscillator strength concomitantly grows in the transparent windows. We clarify that this behavior, related to a third-order nonlinearity, is driven by reverse saturable absorption and is responsible for optical limiting in these compounds [2]. Upon strong incoming fields, incrementally populated dipole- and/or spin-forbidden excitations enhance the absorption in their frequency range while allowed transitions in the linear regime are partially quenched. Our results contribute to the understanding of the fundamental physical mechanisms behind nonlinear light absorption of chromophores.

[1] K. Yabana and G. F. Bertsch, PRB 54, 4484 (1996). [2] C. Cocchi et al., PRL 112, 198303 (2014).

CPP 72: Hybrid and Perovskite Photovoltaics I

Time: Thursday 15:00–18:00 Location: C 264

Invited Talk CPP 72.1 Thu 15:00 C 264

Ionic (in)homogeneity in metal-halide perovskites — •Eva Unger — Helmholtz Zentrum Berlin für Materialien und Energie, Albert Einstein Strasse 16, 12489 Berlin — Lunds Universitet, Naturvetarvägen 14, Lund, Schweden

Metal-Halide Perovskites are highly ionic semiconductors, which gives rise to some intriguing material properties. Alloys with increasing complexity have evolved during the past years in the attempt to tune the material band gap and synthesize perovskite semiconductors with increased stability. In mixed-cation and mixed-anion alloys, ionic (in)homogeneity and photo- or bias-induced ion migration can limit the device performance and give rise to strong transient capacitive effects in current-voltage measurements giving rise to hysteresis. This talk will reflect on ionic (in)homogeneity in metal halide perovskites as it evolves from the complex chemistry in solution to the consequence of ionic entropy on crystallization kinetics and how intrinsic ionic homogeneity or externally induced ion redistribution affect device performance.

CPP 72.2 Thu 15:30 C 264

Interaction of mobile ions and electronic charge carriers in organic-inorganic perovskites revealed by in-situ photoluminescence and Kelvin probe measurements — •Susanne T. Birkhold[1,2], Jake Precht[1], Hongbin Liu[1], Rajiv Giridharagopal[1], Giles E. Eperon[1], Xiasong Li[1], Lukas Schmidt-Mende[2], and David S. Ginger[1] — [1]Department of Chemistry, University of Washington, Seattle, Washington 98195, United States — [2]Department of Physics, University of Konstanz, 78464 Konstanz, Germany

The mixed ionic-electronic conductivity of organic-inorganic perovskites is expected to be responsible for slow response times, current-voltage hysteresis, as well as stoichiometric changes under an electric bias. Here, we present an investigation of the interaction of mobile ions and electronic charges during electric poling of MAPbI3 and FAPbI3. We use in-situ photoluminescence and Kelvin probe microscopy on lateral electrodes to correlate temporal changes in radiative recombination with the spatial distribution of ionic and electronic species. While ion migration is observed using both charge injecting and insulating contacts, our results show that non-radiative recombination centers only form if both ion migration and charge injection are present in MAPbI3. Combining these results with ab initio simulations reveals a complex interaction between ion migration and charge injection that determines defect energetics. Furthermore, temperature dependent SKPM measurements are applied to determine activation energies of ion migration in MAPbI3 and FAPbI3.

CPP 72.3 Thu 15:45 C 264

Capacitance profiling of planar perovskite solar cells taking mobile charged defects into account — •Mathias Fischer[1], Kristofer Tvingstedt[1], Vladimir Dyakonov[1,2], and Andreas Baumann[2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Currently, numerous approaches are being pursued to generate intentionally doped hybrid perovskite semiconducting materials. The Mott-Schottky analysis is a standard method to determine the doping concentration and the built-in potential. It is based on the fact that the depletion layer thickness, and therefore the capacitance changes with an applied electric field. In perovskite solar cells, however, this is typically not the case. We show experimentally that mobile charged defects might lead to erroneous values when not being considered. Instead, charges accumulated at the interface between the perovskite and a transport layer lead to an inhomogeneous doping distribution which is reflected in an underestimated built-in potential and doping density. We present electrical impedance measurements on planar solution-processed methylammonium and formamidinium lead iodide solar cells in a p-i-n configuration. Thereby, we derived a new measurement routine to determine the depletion layer capacitance as well as the doping density and the built-in potential by means of Mott-Schottky analysis. Finally, we provide informations on intentional or unintentional doping profiles in these solar cells.

CPP 72.4 Thu 16:00 C 264

In-Situ Investigation of Ion Migration and Aggregation in Organolead Halide Perovskite Films — •Yu Zhong[1], Carlos Andres Melo Luna[2], Richard Hildner[2], Cheng Li[1], and Sven Huettner[1] — [1]Macromolecular Chemistry I, University of Bayreuth, Bayreuth, Germany — [2]Experimental Phyiscs IV, University of Bayreuth, Bayreuth, Germany

During current-voltage(J-V) measurements, perovskite solar cells(PSCs) exhibit a certain photo-induced instability and hysteresis phenomenon. Firstly, we study the light-induced behavior in CH3NH3PbI3-xClx film in-situ, by employing wide-field photoluminescence(PL) microscopy to obtain both the spatially- and temporally-resolved PL image. Along with the increase of the PL intensity under continuous illumination, some areas render PL inactive. A faster and more obvious PL decay process was observed with a higher excitation energy. By characterizing this excitation energy dependent PL decay, we suggest that the PL quenching can be ascribed to an aggregation of iodide ions. Secondly, by introducing phenyl-C61-butyric acid methyl ester(PCBM) in PSCs, hysteresis phenomenon is suppressed. The results of wide-field PL image and temperature dependent J-V curve measurement confirm that PCBM molecules decrease the mobility and increase the activation energy of iodide ions. This real-time investigation of the light soaking of perovskite films provides more details to improve the performance of PSCs. The suppression of the iodide ions movement, e.g. involving PCBM, is a concern for better performance and stability of PSCs.

CPP 72.5 Thu 16:15 C 264

Correlation of ion migration and charge carrier trap states in organic-inorganic lead halide perovskites — •Susanne Koch, Susanne T. Birkhold, and Lukas Schmidt-Mende — Department of Physics, University of Konstanz, Konstanz, 78457, Germany

While the efficiencies of organic-inorganic perovskite solar cells have seen a strong rise in recent years, the understanding of physical processes inside the material is still limited and devices face stability issues. Many observed phenomena, like current-voltage hysteresis, have been attributed to mobile ions and their interaction with charge carriers. Additionally charge carrier trap states are known to have a strong impact on the carrier dynamics inside the perovskite. Since both ion migration and charge carrier trapping occur simultaneously and are influenced by common material modifications, a correlation between them is possible and could provide information on their origins and contribution to conduction processes. To characterize this possible coupling and to understand electronic and ionic conduction in the perovskite material, the energetic distribution of electronic trap states is studied by measuring thermally stimulated current, while temperature-dependent impedance spectroscopy measurements are employed to extract activation energies for the movement of ionic charges in the material. Using both techniques on comparable systems, where the perovskite is modified targeting specific trap states, should give insights into the correlation of ion migration and trap state distribution.

15 min. break

CPP 72.6 Thu 16:45 C 264

Defect spectroscopy in triple-cation hybrid perovskites — •David Diering[1], Charles Hages[1], Sergiu Levcenco[1], Christian Wolff[2], Dieter Neher[2], and Thomas Unold[1] — [1]Helmholtz-Zentrum Berlin, Germany — [2]Universität Potsdam

High power-conversion efficiencies have been observed for hybrid perovskite solar cells based on multi-cation materials, containing methylammonium (MA), formamidinium (FA), cesium (Cs). Thus, the question arises how the presence of these cations alters the absorbers optoelectronic properties and defect physics. Capacitance spectroscopy such as thermal admittance is an established method to search for defects, which may contribute to non-radiative recombination.

In this study, the impact of cesium incorporation in $(FAPbI_3)_{83}(MAPbBr_3)_{17}$ with cesium contents ranging from 0% to 15% was investigated for a series of solar cells. We performed detailed temperature-dependent admittance measurements, temperature-dependent current-voltage and EQE measurements. The results are correlated with numerical device modelling as well as the opto-electronic properties of the respective pure absorbers, i.e. charge carrier lifetimes.

CPP 72.7 Thu 17:00 C 264

Reducing recombination and enhancing open circuit voltage by Strontium-alloying in multiple cation perovskite solar cells — •Pietro Caprioglio^{1,3}, Fengshuo Zu^{2}, Christian M. Wolff^{1}, Martin Stolterfhot^{1}, Norbert Koch^{2}, Bernd Rech^{3}, Steve Albrecht^{3}, and Dieter Neher^{1} — ^{1}University of Potsdam — ^{2}Humboldt-Universität, Berlin — ^{3}Helmholtz-Zentrum Berlin

State of the art perovskite solar cells still suffer from too low fill factor and open circuit voltage (Voc), which has been related to non-radiative losses mostly happening at the surface. Here, we present the enhancement of the Voc by addition of Strontium (Sr) to a quadruple cation perovskite Rb5(Cs5(MA0.17FA0.83)Pb(I0.83 Br0.17)3)95)95. The resulting material displays significantly enhanced photoluminescence (PL) lifetime and absolute PL yield together with a larger splitting of the quasi-Fermi levels. These findings are confirmed by the increase in Voc and in electroluminescence efficiency observed in actual devices. As a result, the power conversion efficiency increases, reaching a PCE of 20.3% under AM1.5G illumination. We show through various photoelectron spectroscopy techniques (UPS/XPS and IPES), how the addition of Sr induces a more n-type surface and enables better contact selectivity. Such a change in energetics is responsible for a substantial suppression of surface and interface recombination. Morphology characterization shows that Sr is mostly segregated close to the charge transport layers, affecting only the interfaces. In conclusion, we propose that Sr-addition enables an appropriate interface modification that helps to reduce Voc losses.

CPP 72.8 Thu 17:15 C 264

Structural and Compositional Analyses of Perovskite-like Cesium Lead Halides — •Hannah Funk^{1}, Sebastian Caicedo-Davila^{1}, Robert Lovrincic^{2}, Christian Müller^{2}, Michael Sendner^{2}, Frederike Lehmann^{1}, René Gunder^{1}, Alexandra Franz^{1}, Markus Wollgarten^{1}, Benedikt Haas^{3}, Christoph T. Koch^{3}, and Daniel Abou-Ras^{1} — ^{1}Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — ^{2}InnovationLab GmbH, Speyerer Straße 4, 69115 Heidelberg, Germany — ^{3}Humboldt-Universität zu Berlin, Unter den Linden 6, 10099 Berlin, Germany

Inorganic $CsPbX_3$ (X=I, Cl, Br) thin films are investigated as supposedly more stable alternative to methyl-ammonium-containing hybrid perovskite layers for thin-film solar cells. For the present contribution, wide band gap $CsPbBr_3$ thin films were synthesized by spin-coating and coevaporation. In addition, also corresponding powder samples were produced as reference. Structural properties were obtained by X-ray diffraction. To resolve the structure more locally high-resolution images as well as electron diffraction patterns were acquired with a transmission electron microscope. The elemental distributions were analyzed by means of energy-dispersive X-ray spectrometry. The evaluation of these results shows that - in contrast to the powder sample the CsPbBr3 thin films are accompanied by secondary phases such as $CsPb_2Br_5$ or Cs_4PbBr_6. The present contribution will also report on electron beam damage and how to avoid it.

CPP 72.9 Thu 17:30 C 264

Influence of Different Halides and Organic Cations on the Crystallization Dynamics of Perovskite Thin Films — •Alessandro Greco, Alexander Hinderhofer, Jan Hagenlocher, and Frank Schreiber — Institute of Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

The performance of hybrid perovskite thin films in photovoltaic and light emitting devices depends not only on their composition, but also their structural and morphological features.[1] Conventionally, the perovskite thin films in these devices are created with the so-called two-step conversion method, which involves the deposition of an isopropanol solution onto a lead halide precursor (PbX_2, X=I,Br,Cl) via drop casting. The solution contains a defined amount of either methylammonium halide (CH_3NH_3X) or formamidinium halide ($CH(NH_2)_2X$). The morphology and structural properties of perovskites depend strongly on their composition and the crystallization dynamics. We applied in situ grazing incidence wide angle X-ray scattering (GIWAXS) to determine the reaction rate, domain size and preferred orientation in several perovskite thin films over time. We will discuss how choosing different lead halide precursors in combination with different organic halide solutions can impact the quality and time scale of the structural and morphological development of the perovskite thin films.

[1] N. Arora et al. *Science*, **358**, 768 (2017).

CPP 72.10 Thu 17:45 C 264

Topography-dependent phase-segregation in mixed-halide perovskite — •Xiaofeng Tang, Gebhard Matt, and Christoph Brabec — Institute of Materials for Electronics and Energy Technology (i-MEET), Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Mixed-halide perovskites have emerged as promising materials for optoelectronics due to the merit of their tunable bandgap in the entire visible region. A challenge remains however in the instability of the bandgap. This bandgap instability is attributed to phase-segregation, which strongly affects the voltage attained in mixed-halide perovskite-based solar cells and seriously restricts the applications.

In this work, we provide an in-depth insight into this phenomenon with a combination of local-resolved and bulk investigations. We demonstrate phase-segregation in mixed-halide perovskite is topography-dependent. By using spatially-resolved photoluminescence spectroscopy, we show the gradual red-shift of the photoluminescence signal at the grain boundaries of mixed-halide perovskite during the consecutive illumination. Contrarily, we observe the spectrally stable emission exclusively stems from the grain centers. Such difference is further evidenced by bulk characterizations, showing the illuminated mixed-halide perovskite presenting double band-edge features. The above spatially selective halide separation provides a strong argument that ion migration indeed dominantly occurs along these boundaries and will support the development of better passivation strategies, ultimately allowing to process environmentally stable perovskite films.

CPP 73: Functional Polymer Hybrids and Composites

Time: Thursday 15:00–16:30 Location: PC 203

CPP 73.1 Thu 15:00 PC 203

Morphology Control of Low Temperature Fabricated ZnO Nanostructures for All Solid-State Transparent Dye-Sensitized Solar Cells — •Kun Wang^{1}, Volker Körstgens^{1}, Dan Yang^{1}, Nuri Hohn^{1}, Stephan V. Roth^{2,3}, and Peter Müller-Buschbaum^{1} — ^{1}1TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — ^{2}DESY, 22607 Hamburg — ^{3}3KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden

In the last decade dye-sensitized solar cells (DSSCs) have received considerable interest for solar energy conversion due to their convenient and low-cost fabrication. Solid state DSSCs show great promising since they are generally free from electrolyte leakage and corrosion problems compared with the traditional liquid electrolyte solar cells. For the n-type semiconductor ZnO offers higher electron mobility and lower crystallization temperature as compared to titania. A low-temperature route based on a sol-gel method with diblock copolymer templating is demonstrated, through which ZnO films are prepared which have a tunable morphology including foam-like, worm-like and sphere-like structures. The morphologies are probed using SEM and grazing incidence X-ray scattering. Based on the controlled nanostructured ZnO films all solid-state transparent DSSCs are fabricated, which paves the way for building integration of the solar cells.

CPP 73.2 Thu 15:15 PC 203

In-situ GISAXS during sputter deposition of metal nanolayers on functional polymer thin films for lithium-ion batteries — •Simon Schaper^{1}, Franziska C. Löhrer^{1}, Volker Körstgens^{1}, Matthias Schwartzkopf^{2}, Pallavi Pandit^{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 — [2]DESY, 22607 Hamburg — [3]CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, 24143 Kiel

Understanding the interface between metals, commonly used as current collectors, and ion-conducting polymers used in polymer lithium-ion batteries (LIBs) is crucial to develop highly reproducible, low-cost and reliable devices. To address these issues, sputter deposition is the technique of choice to fabricate scalable, reproducible and controllable nanometer and sub-nanometer metal layers on polymer thin films. The sputter deposition process, being well understood and controlled, offers advantages over chemical methods to tailor metal thin-flim morphologies on the nanoscale and offers a superior adhesion of the deposited material.[1] We use in-situ grazing incidence small angle X-ray scattering (GISAXS) to investigate the formation, growth and self-assembled structuring on polymer thin films used in LIBs.[2] Different polymer films are compared with respect to the metal layer growth.

[1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 9, 5629 (2017);

[2] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015).

CPP 73.3 Thu 15:30 PC 203

Characterization of gold nanoparticle loading and distribution within polymer brushes by neutron reflectometry — •Dikran Kesal[1], Larissa Braun[1], Oliver Löhmann[1], Emanuel Schneck[2], Marcus Trapp[3], and Regine von Klitzing[1] — [1]Soft Matter at Interfaces, Department of Physics, TU Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt, Germany — [2]Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14476 Potsdam, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Polymer brushes are promising candidates for the design of smart surfaces. Exposed to specific stimuli, these systems undergo structural changes. Furthermore, they can be used as a matrix for the uptake of particles. Incorporating gold nanoparticles (AuNPs) in polymer brushes results in nanocomposite materials with interesting nanosensor properties due to the fact that AuNPs exhibit surface plasmon resonance (spr). Here, the interparticle distance can be used to shift the spr in a certain way. The aim is to correlate the AuNP distribution with optical properties. In the present study neutron reflectometry is used for studying the distribution of AuNPs.

The focus is on the concentration profile of AuNPs within the polymer brush, which were incubated at different pH values. The sensitivity of the method is enhanced by the use of contrast variation. The reflectivity data are analyzed with a self-written fitting procedure based on volume fraction profiles of all chemical components.

CPP 73.4 Thu 15:45 PC 203

Influence of particle microstructure on the effect of magnetostriction in magneto-sensitive elastomers — •Dirk Romeis, Vladimir Toshchevikov, and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden e.V.

Magneto-sensitive elastomers (MSEs) are field-controllable composite materials with magnetically switchable properties. They consist of a soft-elastic polymer network with immersed magnetizable microparticles. Under external magnetic field these composites can significantly change their mechanical properties. Recently, we developed a dipolar mean field approach [1] to predict the effective material behavior of MSE in the magnetic field. Especially for random isotropic distribution of the magnetizable particles we find a quantitative agreement with micro-scale continuum simulations [2]. Presently, the mean field approach is limited to special situations, such as a conservation of the particle microstructure and specific orientation of the magnetic field. However, for ultra-soft elastomer we expect the particles to rearrange into different structures if the external field is applied. We will present some modifications in order to describe the mechanical behavior of MSEs under more general conditions. This will help us to gain an enhanced understanding of this type of field-controllable polymer composites. This work was supported by DFG (Project GR 3725 / 7-2).

Literature

[1] *Romeis D. et. al.* Soft Matter **12**, 9364-9376 (2016)

[2] *Romeis D. et. al.* Physical Review E **95**, 042501 (2017)

CPP 73.5 Thu 16:00 PC 203

Density functional theory for ferrogels and magnetorheological elastomers — Peet Cremer[1], Marco Heinen[2], •Andreas M. Menzel[1], and Hartmut Löwen[1] — [1]Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany — [2]Universidad de Guanajuato, Guanajuato, Mexico

Locking the positions of magnetic or magnetizable colloidal particles in an elastic polymer matrix leads to an interesting class of composite materials. One remarkable feature is that their overall mechanical properties can be reversibly tuned from outside by magnetic fields.

Our scope was to establish a statistical approach to this situation in terms of classical density functional theory, including thermal fluctuations [1]. To lower the complexity, we mapped the problem to a suitable one-dimensional dipole-spring model. A central issue is that classical density functional theory was constructed to describe liquid-like states, in contrast to our fixed particle positions in the elastic matrix. We solved this problem by introducing suitable particle pair and external potentials to mimic corresponding elastic interactions. Comparison with Monte-Carlo simulations showed good agreement. In parts, the theory uses input from explicit analytical calculations of the elastic response of the polymer matrix [2,3].

The theory allows to calculate, for instance, the change in the elastic modulus for varying strengths of the magnetic particle interactions.

[1] P. Cremer et al., *J. Phys.: Condens. Matter* **29**, 275102 (2017).

[2] M. Puljiz et al., *Phys. Rev. Lett.* **117**, 238003 (2016).

[3] M. Puljiz et al., *Phys. Rev. E* **95**, 053002 (2017).

CPP 73.6 Thu 16:15 PC 203

Photodegradation Evaluation in PVC Films and Resonance Raman Spectroscopic Insights into the Patterns of UV Light-Induced Polyene Defects — •Patrice Donfack[1], Elena A. Sagitova[2], Gulnara Yu. Nikolaeva[2], Alexandra Costa[3], Simon J. Shilton[3], Dmitry I. Mendeleyev[4], Kirill A. Prokhorov[2], and Arnulf Materny[1] — [1]Jacobs University, Bremen, Germany — [2]A.M. Prokhorov General Physics Institute of the Russian Academy of Sciences, Moscow, Russia — [3]University of Strathclyde, Glasgow, Scotland, UK — [4]A.V. Topchiev Institute of Petrochemical Synthesis of Russian Academy of Sciences, Moscow, Russia

Polyvinylchloride (PVC) is among the most popular components in modern industrial composite polymer materials, whose structure can be purposefully tuned within a wide range to feature new interesting physical and chemical properties. Typical application-relevant properties of PVC-based materials are affected by the formation of conjugated double bond defects (polyene) as the result of e.g. mechanical, thermal, chemical, or optical factors. In the present contribution, the PVC structure and especially the UV irradiation-induced polyene formation in the PVC matrix are studied using a combination of several techniques, including resonance Raman spectroscopy. The latter has proven very powerful in providing structural insights in both the small crystalline and the predominantly amorphous phases in PVC. Our results uncover the size distribution and content of polyene defects in a photodegraded PVC matrix as a function of UV-irradiation doses, yielding important information relevant for PVC-based insulating materials.

CPP 74: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VII (joint session O/TT/MM/DS/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France Paul R. Kent, Oak Ridge National Laboratory, USA Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Thursday 15:00–17:45 Location: HL 001

Invited Talk CPP 74.1 Thu 15:00 HL 001

Recent developments in FCIQMC: real-time propagation and improved convergence with walker number — •Ali Alavi — Max Planck Institute for Solid State Research, Stuttgart, Germany

The Full Configuration Interaction QMC method samples Slater determinants using an imaginary-time propagation of walkers, and can yield essentially exact ground- and excited states energies and wavefunctions for Fermionic systems. Recently we have extended this methodology to real-time propagation, enabling the calculation of spectral functions along the real-frequency axis. This method will be described in the talk, together with representative examples from molecular and lattice models. We will also describe a second development in the FCIQMC methodology which substantially improves the rate of convergence of the ground-state technique with respect to the number of walkers. With the new method, we can compute essentially the exact ground state energy of the benzene molecule, correlating 30 electrons (the entire valence) in the full set of 108 orbitals of a VDZ basis. Perspectives of the new methods will be discussed.

CPP 74.2 Thu 15:30 HL 001

Quasi-Continuous LDA+DMFT calculations for SrVO3. — •Evan Sheridan, Christopher Rhodes, Evgeny Plekhanov, and Cedric Weber — King's College London, Theory and Simulation of Condensed Matter (TSCM), The Strand, London, United Kingdom.

The Dynamical Mean Field Theory (DMFT) is an extremely powerful tool in the treatment of strongly correlated electron systems and many DMFT calculations suffer from a computational bottleneck when it attempts to solve the Anderson Impurity Model (AIM).

Common among the early Anderson Impurity solvers was the Auxiliary Field Quantum Monte Carlo (AF-QMC) approach which relies on a discretisation of the imaginary time grid. AF-QMC solvers suffer from the notorious Suzuki-Trotter error,as a result of this , that has largely been ignored in recent years with the advent of Continuous Time-QMC (CT-QMC) solvers.

Here, we present a systematic study of how this issue can be overcome for realistic material properties using LDA+DMFT. We find that our quasi-continuous time method compares well to the state-of-the-art CT-QMC calculations for SrVO3, with the added advantage of linear scaling in temperature. The theoretical framework proposed is quite general and can be extended to cluster DMFT calculations.

CPP 74.3 Thu 15:45 HL 001

High temperature superconducting oxychlorides: a light element model for cuprates — •Matteo d'Astuto[1,2], Blair Lebert[2,3], Ikuya Yamada[4], and Masaki Azuma[5] — [1]Institut NEEL CNRS/UGA UPR2940 25 rue des Martyrs BP 166 38042 Grenoble cedex 9 FRANCE — [2]IMPMC, UMR7590 UPMC-Sorbonne Universités - CNRS, Paris, France — [3]Synchrotron SOLEIL, Gif-sur-Yvette, France — [4]Nanoscience and Nanotechnology Research Center (N2RC), Osaka, Japan — [5]Materials and Structures Laboratory, TITech, Yokohama, Japan

The copper oxychloride cuprate $Ca_2CuO_2Cl_2$ (CCOC) system, with vacancy or Na doping on the Ca site, is unique among the high temperature superconducting cuprates (HTSCs) since it: lacks high Z atoms; has a simple I4/mmm 1-layer structure, typical of 214 (LSCO) cuprates, but which is stable at all doping and temperatures; and has a strong 2D character due to the replacement of apical oxygen with chlorine. It also shows a remarkable phase digram, with a superconducting T_C growing to the optimal doping without any minimum around 1/8 doping, despite the observation of charge modulations by near-field spectro-microscopy. Due to the reduced number of electrons, advanced calculations that incorporate correlation effects, such as quantum Monte Carlo are easier, but relatively little is known about CCOC (for a cuprate) from an experimental point of view. We are now filling this gap by a comprehensive experimental study covering the whole phase diagram, in particular of the (para)magnon and phonon dispersion..

CPP 74.4 Thu 16:00 HL 001

Antiferromagnetic correlations in the metallic strongly correlated transition metal oxide $LaNiO_3$ — •Hanjie Guo[1], Zhiwei Li[1], Li Zhao[1], Zhiwei Hu[1], Chunfu Chang[1], Changyang Kuo[1], Wolfgang Schmidt[2], Andrea Piovano[2], Tunwen Pi[3], Oleg Sobolev[4], Daniel Khomskii[1], Liu Hao Tjeng[1], and Alexander Komarek[1] — [1]MPI CPfS, Dresden, Germany — [2]ILL, Grenoble, France — [3]NSRRC, Taiwan — [4]FRMII, Munich, Germany

The material class of rare earth nickelates with high Ni^{3+} oxidation state is generating continued interest due to the occurrence of a metal-insulator transition with charge order and the appearance of non-collinear magnetic phases within this insulating regime. The recent theoretical prediction for superconductivity in $LaNiO_3$ thin films has also triggered intensive research efforts. $LaNiO_3$ seems to be the only rare earth nickelate that stays metallic and paramagnetic down to lowest temperatures. So far, centimetre-sized impurity-free single crystal growth has not been reported for the rare earth nickelates material class since elevated oxygen pressures are required for their synthesis. Here, we report on the successful growth of centimetre-sized $LaNiO_3$ single crystals by the floating zone technique at oxygen pressures of up to 150 bar. Our crystals are essentially free from Ni^{2+} impurities and exhibit metallic properties together with an unexpected but clear antiferromagnetic transition.

CPP 74.5 Thu 16:15 HL 001

First-principles quantum Monte Carlo study of correlated materials — •Huihuo Zheng — Argonne Leadership Computing Facility, Argonne National Laboratory, Lemont, USA

Strongly correlated electronic systems have become an important subject of condensed matter physics, because of many fascinating phenomena arising in these systems such as metal-insulator transition, high temperature superconductivity, etc. Accurate characterization of the electron-electron correlations in these systems from first principles is essential for us to understand how these phenomena emerge from microscopic interactions. I will present our efforts in modeling correlated materials using the first-principles quantum Monte Carlo (QMC) method by showing two representative *ab intio* studies (vanadium dioxide and graphene) and a density-matrix downfolding theory for constructing low energy effective models from *ab initio* simulations. Using QMC, we correctly characterized the electronic structure of vanadium dioxide and unveiled the electronic origin of the metal-insulator transition which has been a mystery for decades. For graphene, we computed the electron screening from σ bonding electrons and illustrated how the emergent physics from underlying Coulomb interactions results in the observed weakly correlated semimetal. On the other hand, the downfolding approach we developed provides a way to quantitatively identify important microscopic interactions relevant to the macroscopic physics.

CPP 74.6 Thu 16:30 HL 001

Reduced Density Matrix Theory for Coupled Fermion-Boson Systems — •Florian Buchholz[1], Iris Theophilou[1], Michael Ruggenthaler[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]MPSD, Hamburg, Germany — [2]CCQ, The Flatiron Institute, New York, United Sates — [3]Nano-bio Spectroscopy Group, San Sebastián, Spain

Reduced density matrix (RDM) theory proved to be successful in describing a wide range of many-body problems that are not easily accessible by the more common many-body perturbation theories or density functional theory. Especially as RDM theories are non-perturbative, they are advantageous in strong coupling scenarios.

However, RDM theory was to our knowledge never applied to systems with more than one active particle type. The focus of this talk is to analyze the possibilities and problems of an extension to coupled fermion-boson theories. Comparing a typical bilinear interaction term of the form $c_i^+ c_j(a_k^+ + a_k)$, where c^+/c and a^+/a indicate fermion and boson creation/annihilation operators, respectively and the fermionic 2-body interaction term $c_i^+ c_j^+ c_k c_l$, the former should have a considerably reduced definition space, which we hope to be exploitable. On the other hand, the bilinear interaction has a very different structure than the 2-body interaction and it is not clear at all, how to define a RDM that carries all information to compute experimental observables of a coupled fermion-boson system.

Specifically, I will illustrate some of the peculiarities of the fermion-boson interaction for simple model systems and present some ideas to deal with those.

CPP 74.7 Thu 16:45 HL 001

Critical temperatures as function of magnetic anisotropy in two-dimensional systems from first-principles calculations — •Daniele Torelli — Center for Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

Recent observation of ferromagnetic out-of-plane order in monolayer CrI_3 highlights the importance of a microscopic understanding of anisotropy in ground state magnetic systems. Single-ion anisotropy accounts mainly for spin-orbit coupling interaction and, in particular for two-dimensional (2D) materials, it's crucial to escape the Mermin-Wagner theorem. Here we investigate the variation of critical temperatures as functions of anisotropy in Heisenberg model systems using Metropolis Monte Carlo simulations. Results for square, hexagonal and honeycomb lattices are compared with equivalent simulations in the Ising model, which is confirmed to represent the limit with infinite anisotropy. Based on a new developed computational 2D materials database, we predict a vast number of 2D structures with high critical temperatures. As testing system, relevant Heisenberg exchange couplings and magnetic anisotropy energy in CrI_3 monolayer are extracted from first principle calculations and energy mapping analysis, yielding to an estimation of Curie temperature in good agreement with experimental results.

CPP 74.8 Thu 17:00 HL 001

Oxygen vacancy-induced absorption of visible light in SrNbO3 — •Marcello Turtulici, Steffen Backes, and Silke Biermann — Centre de Physique Théorique, Ecole Polytechnique, 91128 Palaiseau, France

SrNbO3 has recently attracted attention as a bright red photocatalyst. Several, mutually contradicting, models have been proposed in the literature in order to explain the strong absorption in the visible spectrum, and no consensus even on the basic nature of the mechanism has been reached. In this work we investigate the optical properties of this material by means of state-of-the-art Density Functional Theory and many-body perturbation theory techniques. We evidence a high sensitivity of the optical properties on deviations from the ideal crystal structure. In particular, the optical properties should strongly depend on the presence of oxygen vacancies, which give rise to additional absorption channels in the visible frequency range. Most notably, the experimentally observed red color is likely due to transitions between orbitals of dominant Nb-eg character, which are enhanced by the strong hybridization of the quite extended 4d-states of Nb with oxygen p-states.

CPP 74.9 Thu 17:15 HL 001

Transient charge and energy flow in the wide-band limit — Fabio Covito, •Florian Eich, Riku Tuovinen, Michael Sentef, and Angel Rubio — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Thanks to recent advances in ultra-fast pump-probe spectroscopies and nano-thermometry it is possible to study charge and energy flow at atomic time and length scales. In order to analyze the transient dynamics of nanoscale devices theoretically, the wide-band limit is a commonly used approximation. Here we investigate the applicability of the wide-band limit to the study of charge and heat transport through nanojunctions exposed to voltage biases and temperature gradients. We find that while this approximation faithfully describes the long-time steady-state charge and heat transport, it fails to characterize the short-time transient behavior of the junction. In particular, we find that the charge current flowing through the device shows a discontinuity when a temperature gradient is applied, while the energy flow is discontinuous when a voltage bias drives the dynamics and even diverges when the junction is exposed to both a temperature gradient and a voltage bias. We discuss this pathological behavior and propose two possible solutions.

CPP 74.10 Thu 17:30 HL 001

From DFT to Coupled Cluster Theory - Understanding Oxygen Activation on Coin Metal Nanoparticles — •Wilke Dononelli and Thorsten Klüner — Institut für Chemie, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

In this study we focus on one of the most fundamental catalytic model reactions, the oxidation of CO on a metal catalyst. We studied the activation of molecular oxygen via dissociation or direct reaction of CO and O_2 within density functional theory (DFT) and high level CCSD(T) calculations. Therefore we use Au_{13} and Au_{55} nanoparticles (NPs) and a periodic Au(321) surface as model systems and compare the catalytic activity of the gold substrates to Ag and Cu based, as well as bimetallic NP catalysts. Part of the DFT calculations were performed, using the well-established PBE functional as implemented in the Vienna ab initio simulation package (VASP). Hybrid and double hybrid DFT calculations on the NPs were performed in Gaussian09. CCSD(T) calculation were performed in Gaussian09 using conventional CCSD(T) for the M_{13} (M=Au,Ag,Cu) NPs and CCSD(T)/PBE in a QM/QM embedding scheme using the ONIOM approach for M_{55} NPs. For systems of 55 metal atoms PBE gives the same results as double hybrids or even CCSD(T). For smaller M_{13} NPs interaction energies differ between PBE and higher levels of theory, which might be explained by the molecule like character of these NPs.

CPP 75: Annual General Meeting of the CPP Division (CPP Mitgliederversammlung)

Time: Thursday 18:45–19:45 Location: C 130

Duration 60 min.

CPP 76: Focus: Polymers in Multi-Compartment and Aqueous Solutions II - organized by Jens-Uwe Sommer and Debasish Mukheri

Time: Friday 9:30–11:30 Location: C 130

Topical Talk CPP 76.1 Fri 9:30 C 130

Optimal inhibition and spatial organization of irreversible protein aggregation using liquid compartments — •Christoph A. Weber[1,2], Thomas Michaels[1], and L. Mahadevan[1] — [1]Harvard John A. Paulson School of Engineering and Applied Science, Cambridge — [2]Max Planck Institute for the Physics of Complex Systems, Dresden

Protein aggregation in cells is an ubiquitous phenomenon and linked to a large variety of diseases, such as Alzheimer's and Parkinson's disease, amyloidosis or type II diabetes. So far, there is no effective strategy to suppress or inhibit protein aggregation in these systems. Typically, it has been suggested to design drugs which stabilize monomers against aggregation, or block the surface or the ends of aggregates. We show that this treatment strategy can be optimized increasing dramatically the life time of the cell. In addition, we suggest a novel strategy, namely to spatially segregate protein aggregation in distinct liquid-like cellular compartments in a controllable fashion. Many cells actually use droplet-like compartments to spatially organize the cellular cytoplasm but only little is known about their biological function. Here, we show that liquid compartments are ideally suited to spatially organize protein aggregation. Aggregation only occurring in these compartments keeps the toxic aggregates away from the sensible intracellular surrounding and allows subsequent localized and specific degradation by the cellular machinery or drugs. Since the compartment assembly creates costs we employ optimal control theory to determine the optimal physical parameter for spatial segregation of protein aggregation.

CPP 76.2 Fri 10:00 C 130

Molecular insights into the temperature-induced transition of Poly(N-n-propylacrylamide) (PNnPAm) in aqueous solution. — •Tiago Espinosa de Oliveira[1], Carlos Marques[1], and Paulo Netz[2] — [1]Institut Charles Sadron, CNRS, Strasbourg, France — [2]Universidade Federal do Rio Grande do Sul, Proto Alegre, Brazil

The possibility of tuning the molecular structure of smart polymers increases the potential of technological applications of these materials. In this context, N-substituted acrylamide-based polymers exhibit a drastic phase transition by slight changes in temperature. Moreover, Poly(N-n-propylacrylamide) (PNnPAm) and Poly(N-isopropylacrylamide) (PNIPAm) are polymers which exhibit a lower critical solution temperature (LCST) at 297 and 305 K, respectively. Furthermore, PNnPAm exhibits a sharp and discontinuous phase transition in aqueous solution, in contrast to PNIPAm. In this work, we carried out all-atom molecular dynamics simulations to understand, from a microscopic point-of-view, the influence of chain size and concentration on the LCST of PNnPAm compared to PNIPAm. Our analysis not only shows that the chain length has a strong influence on the LCST but allows also to discriminate the role of the hydration and intramolecular interactions in the collapsing transition.

CPP 76.3 Fri 10:15 C 130

Implicit-solvent coarse-grained models of thermoresponsive polymers — •Richard Chudoba[1,2], Jan Heyda[3], and Joachim Dzubiella[1,2] — [1]Inst. für Physik, Humboldt-Universität zu Berlin, Germany — [2]Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Germany — [3]Dept. of Physical Chemistry, University of Chemistry and Technology, Prague, Czechia

Thermoresponsive polymers have become an integral building block for the development of 'smart', environment-sensitive materials with tunable properties. In particular close to their lower-critical solution temperature (LCST), those polymers show dramatic changes in their physicochemical properties, in response to only tiny changes in the solvent environment, e.g., salt concentration.

Here, we develop and employ a coarse-graining strategy for explicitly temperature-dependent implicit-solvent models of thermosensitive polymers in aqueous solution that are applicable in a wide temperature range, including the crossing of the LCST. We combine both bottom-up and top-down approaches, i.e., atomistic simulations coupled with the iterative Boltzmann inversion method and adjustment of the force field parameters based on the experimental data, to faithfully capture structural and thermodynamic properties of the thermoresponsive polymers. Our primary target is polyethylene glycol (PEG), a versatile polymer in soft material development.

- Chudoba, R.; Heyda, J.; Dzubiella, J. Temperature-Dependent Implicit-Solvent Model of Polyethylene Glycol in Aqueous Solution. J. Chem. Theory Comput. 2017, doi: 10.1021/acs.jctc.7b00560.

CPP 76.4 Fri 10:30 C 130

Upper Critical Solution Temperature (UCST)-type Thermoresponsive Polymers from Hydrogen-Bonding Monomers — Asad Asadujjaman[1], Vahid Ahmadi[1], and •Annabelle Bertin[1,2] — [1]German Federal Institute for Materials Research and Testing (BAM), Dpt. 6 Materials Protection and Surface Technologies, Unter den Eichen 87, 12205 Berlin, Germany — [2]Freie Universität Berlin, Institute of Chemistry and Biochemistry, Takustr. 3, 14195 Berlin, Germany

UCST-type thermoresponsive polymers (i.e. that phase separate from solution upon cooling) present a tremendous potential not only in aqueous media where they can be used in drug delivery, diagnostic and microfluidic applications, but also in water/alcohol mixtures, where they can be used for instance in sensing systems for alcohol-soluble drugs. However, only a few thermoresponsive polymers have been reported that present an UCST in a relevant temperature range and "green" solvents such as water or ethanol. In this context, acrylamide-based monomers can be very useful building blocks for designing novel nonionic UCST-type polymers because of their hydrophilic nature (with the appropriate side chain) and propensity to form hydrogen bonds. We will present our latest results on the UCST-type thermoresponsive behaviour of acrylamide- and 2,6-diaminopyridine-based homopolymers and copolymers in water or water/alcohol mixtures, and give some insights about the rational design of UCST polymers relying on H-bonding.

CPP 76.5 Fri 10:45 C 130

Molecular Dynamics simulations of strain-induced phase transition of poly(ethylene oxide) in water — •Sergii Donets[1], Olga Guskova[1], and Jens-Uwe Sommer[1,2] — [1]Institute Theory of Polymers, Leibniz-Institute of Polymer Research, D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany

An aqueous solution of poly(ethylene oxide) (PEO) oligomers is considered as a potential candidate capable of undergoing a phase transition as a result of loss of the hydrated structure. Our simulations using an atomistic model for PEO and water clearly indicate that an elongating force dipole acting on both chain ends of oligomer chains initiates interchain aggregation with the formation of highly oriented fibrillar nanostructures. The strain-induced demixing transition occurs primarily due to the favorable van der Waals interactions between the PEO chains. A tensile stress introduced into the aqueous solution of PEO changes the solvent quality from good to poor as a function of conformational state of the chains and, if there are other oligomer chains present in the simulations box, leads to a phase separation of PEO from water. The strain-induced demixing of the extended PEO chains provides the possibility to obtain polymer fibers with low energy costs.

Topical Talk CPP 76.6 Fri 11:00 C 130

Diffusion of proteins in bicontinuous microemulsions: controlled soft nano-confinement — •Thomas Hellweg, Oliver Wrede, and Ralph Neubauer — Physikalische und Biophysikalische Chemie, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany

The interior of cells is crowded with different objects and the diffusive behaviour of proteins often does not follow the normal Fick type diffusion, where the mean square displacement grows linearly in time $\langle x^2 \rangle \propto t$. The diffusion is considered to be sub-diffusive if $\langle x^2 \rangle \propto t^\alpha$ (with $\alpha < 1$) [1]. However, due to the complexity of the cellular matrix it is very difficult to control the crowding conditions or the confinement and to make systematic studies inside living cells. Hence, to better understand the dependence of protein diffusion on a confining environment, we study the movement of a fluorescent protein (GFP+) through bicontinuous microemulsions via FCS. The sponge like microemulsion structure, which is characterized via small angle scattering, not only slows down the translational movement of the tracer particle with decreasing domain size but also changes the characteristics of the diffusion from "Fick like" to "anomalous"[1]. Additional relevance for such works arises due to the use of microemulsions as reaction media for enzymatically catalyzed reactions [2].

[1]R. Neubauer, S. Höhn, M. Dulle, A. Lapp, C. Schulreich, and T. Hellweg, Soft Matter 13 (2017), 1998
[2]S. Wellert et al., Euro. Biophysics J., 40 (2011) 761

CPP 77: Organic Electronics and Photovoltaics - Transport and Doping

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

Invited Talk CPP 77.1 Fri 9:30 C 243
High-Performance Organic Transistors — •Karl Leo — IAPP, TU Dresden, 01062 Dresden

Organic field effect transistors (OFET) have so far not achieved major commercial impact, despite their many attractive properties such as low-cost, low-temperature processing, and flexibility. In this talk, I will discuss recent work which addresses some of the shortcomings of the OFET. One key approach is to introduce controlled electrical doping into OFET structures /1/. We have recently shown /2,3/ that this allows for the first time the realization of organic inversion transistors. Furthermore, I will discuss vertical transistor structures which have very short channel length without micropatterning. These structues allow much higher current densities than the lateral OFET despite rather simple processing technology without high-resolution patterning /4,5/. These devices are well suited to drive organic light emitting diodes (OLED), allowing all-organic flexible OLED displays. Recently, we have achieved current densities as high as kA/cm 2 and frequencies above 30MHz /6/.

/1/ K. Walzer et al., Chem. Rev. 107, 1233 (2007) /2/ B. Lüssem et al., Nature Comm. 4, 2775 (2013) /3/ A.A. Guenther et al., APL 106, 233301 (2015) /4/ A. Fischer et al., Appl. Phys. Lett. 101, 213303 (2012) /5/ M.P. Klinger et al., Adv. Mat. 27, 7734 (2015) /6/M. P. Klinger et al., Nat. Sci. Rep. 7, 4471 (2017)

CPP 77.2 Fri 10:00 C 243
How does molecular structure influence charge mobility? - Mining a database of organic semiconductors. — •Christian Kunkel, Christoph Schober, Johannes Margraf, Karsten Reuter, and Harald Oberhofer — Technische Universität München

Improving charge carrier mobilities in organic semiconductors is a challenging task, usually tackled by structural tuning of a promising compound family, while relying on intuition or experience. Still, the vast chemical space is then only locally explored, while promising design strategies might also be uncovered from systematic analysis of large compound databases. We carry out such an analysis by applying charge carrier mobility simulations and data mining strategies to an inhouse database of $>$ 64.000 organic crystals, obtained from the Cambridge Structural Database (CSD) and screened for charge transport properties using first principle derived descriptors. The analysis shows, that our screening recovers many known and well performing materials, while also finding many promising candidates, not yet considered for organic electronics applications. To further derive design principles from the data, we evaluate the intrinsic suitability of $\approx$ 200 molecular scaffolds found to be contained as compound-clusters in our database. A similarity network analysis hints at already explored regions of chemical space, while statistical analysis of the clusters uncovers significant expectable performance differences. Such information can be the basis for further in-depth theoretical and experimental design of materials for organic electronics, highlighting the value of data-based approaches.

CPP 77.3 Fri 10:15 C 243
Charge transport of thiophene containing D/A small conjugated molecules and monomer in π-π isolated stacks — •Deyan Raychev[1,2], Gotthard Seifert[1,3], Jens-Uwe Sommer[1,2,4], and Olga Guskova[1,2] — [1]DCMS, TU Dresden — [2]Leibniz IPF Dresden — [3]Theoretical Chemistry, TU Dresden — [4]Institute for Theoretical Physics, TU Dresden

A lot of effort has been done in order to improve the performance of organic electronics devices. Since the charge transport (CT) in technology relevant materials is a multiparametric problem, it is very challenging task to predict these properties in computer simulations. Here, we investigate CT properties of benzothiadiazole (BTZ) and diketopyrrolopyrole (DPP) based molecules linked with thiophene (Th) as a flaking unit and their monomer (Th-BTZ-Th, Th-DPP-Th and Th-BTZ-Th-DPP-Th) in segregated and mixed π-π stacks using DFT and semiclassical Marcus theory. Scanning the potential surface of the molecules in stacks, we found out that the configurations with minimal binding energies are very close to the experimental crystal structures. For such mixed π-π isolated stacks, the hopping mobilities are calculated and compared with experimental data. Interestingly, the predicted values are very close to the measured mobilities for polymer [1] and molecular crystals [2, 3].

This work is supported by ERDF and Free State of Saxony via ESF project 100231947. [1] P. Sonar et. al., Adv. Mater., 2010, 22, 5409-5413. [2] P. B. Pati et. al., ACS Appl. Mater. Interfaces, 2013, 5, 12460-12468. [3] J. Dhar et. al., Chem. Commun., 2015, 51, 97-100.

CPP 77.4 Fri 10:30 C 243
Measuring the Lateral Charge-Carrier Mobility in Metal-Insulator-Semiconductor Capacitors via Kelvin-Probe — •Karl-Philipp Strunk[1], Valeria Milotti[1], Alexander Ullrich[2], and Christian Melzer[1] — [1]Centre for Advanced Materials, University of Heidelberg, Germany — [2]Organisch-Chemisches Institut, University of Heidelberg, Germany

DC current-voltage measurements on organic field-effect transistors are commonly used to characterize the planar electrical transport in organic semiconductors. We have reported an alternative AC dark-injection method giving access to in-plane transport parameters of organic semiconductor thin films. Exposing a metal-insulator-semiconductor structure to a periodic bias leads to a periodic change in surface potential which can be tracked via a Kelvin-Probe giving direct insight into the movement of lateral charge-carrier waves along the organic film. Based on a simple model the charge-carrier mobility of the semiconducting layer can be extracted from experimental data. In this study we further investigate the validity of the proposed model via two dimensional finite-element simulations. We investigate the influence of properties like doping concentration, traps states and applied bias on the device response. It is found that the model predicts the surface potential oscillations very well for a wide range of parameters. Ad-hoc expansions of the model to include additional effects such as doping and traps states further increase its accuracy, giving it a broad applicability if accurate experimental measurements of the mobility are needed.

CPP 77.5 Fri 10:45 C 243
Studying the Mobility of Metal-Organic Frameworks — •Christoph Muschielok and Harald Oberhofer — Technische Universität München, Germany

Metal-Organic Frameworks (MOFs) are artificial, self-assembled networks of metal centers connected by organic linker molecules. They exhibit large pores, into which small molecules may be absorbed. This structural feature can be exploited in a hypothetic MOF-based trace gas surface acoustic wave (SAW) sensor. Such a device needs – from a theorist's point of view – a profound knowledge of the charge carrier mobility and density within MOFs.

Contrary to most MOFs the class of metal triazolates, notably iron-(II)-triazolate, have quite recently been found to show promising conductive properties. It is now crucial to understand why in particular these compounds have such a high mobility compared to other MOFs. Therefore, we study the applicability of different charge transport (CT) models to the mobility of the charge carriers in metal triazolates based mainly on density-functional theory (DFT).

Starting from there, we also focus on the development of general design principles for semiconducting MOF materials. These can provide guidelines for MOF synthesis to ultimately enable the tayloring of MOF properties to a variety of specific use-cases.

15 min. break

CPP 77.6 Fri 11:15 C 243

Band bending in crystalline silicon induced by molecular doped P3HT — •Matthias Zellmeier, Mathias Mews, Dorothee Menzel, Lars Korte, and Jörg Rappich — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Kekuléstr. 5, 12489 Berlin, Germany

Molecular doping of the organic semiconductor poly-(3-hexylthiophene), P3HT, with the strong molecular acceptor 2,3,5,6-tetrafluorotetracyano-quinodimethane, F4TCNQ, is one of the most common techniques to overcome the restriction of low conductivity in this organic material. The well-established method leads to a decrease of the hole mobility in the low-to-medium doping regime, while the hole density increases linearly with the doping concentration. Additionally, it presents an important prerequisite towards controlling p/n-junctions involving organic materials. Hybrid interfaces combining organic materials and inorganic semiconductors are of special importance as they are crucial for the performance of most applications, e.g. light emitting devices or solar cells. Employing photoelectron spectroscopy, we studied the interface between crystalline silicon, c-Si, and doped P3HT. The doping in the spin coated organic layer was varied from a low doping concentration of 1:1000 F4TCNQ molecules per 3HT monomer units up to 1:3. UPS was used to monitor the development of the HOMO-onset upon doping as well as the work function. A special focus is placed on the shift of the silicon 2p orbital binding energy, which is measured using XPS. The data is used to extract the band bending at the silicon/organic semiconductor junction.

CPP 77.7 Fri 11:30 C 243

Doping of Semiconducting Polymers: Structural Order and Dopant Drift — •Lars Müller[1,2,3], Sebastian Beck[1,3], Wenlan Liu[1,4], Annemarie Pucci[1,3], Andreas Köhn[4], Wolfgang Kowalsky[1,2,3], and Robert Lovrincic[1,2] — [1]InnovationLab, Heidelberg, Germany — [2]Institute for High-Frequency Technology, TU Braunschweig, Germany — [3]Kirchhoff Institute for Physics, Heidelberg University, Germany — [4]Institute for Theoretical Chemistry, University of Stuttgart, Germany

Electrical doping of organic semiconductors is widely applied to fabricate high performance organic electronic devices. First, this contribution studies the electric-field-induced drift of molecular dopants for different host-dopant combinations and the influence of structural order on this drift [1]. Second, we present a study that focuses on the spatial position of dopant molecules in P3HT crystallites, together with a DFT-based approach that can explain the observed changes in π-π lattice spacing without the need for a dopant intercalation. The drift study includes Poly(3-hexylthiophene-2,5-diyl) (P3HT) doped with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ), as well as larger dopant molecules and different host materials. We find that the dynamic drift-process can be utilized to deliberately create highly doped and almost undoped regions within one thin film, resulting in a spatially altered conductivity. The applicability is shown on proof-of-principle memristive devices that are based on this effect.

[1] L. Müller et al., *Adv. Mater.* 2017, 1701466.

CPP 77.8 Fri 11:45 C 243

Quantitative Molecular Doping and Electron Trapping in Single-Wall Carbon Nanotubes — •Michael Auth[1], Bernd Sturdza[1], Klaus H. Eckstein[2], Florian Oberndorfer[2], Andreas Sperlich[1], Tobias Hertel[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Institute of Physical and Theoretical Chemistry, Julius Maximilian University of Würzburg, 97074 Würzburg — [3]Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

Defects and doping in Single-Wall Carbon Nanotubes (SWNTs) by (electro-) chemical methods is a highly important topic for future applications of SWNTs. Previous indirect all-optical techniques hypothesise charge carrier localisation in SWNTs due to adjacent $AuCl_3$ molecules, which is indicated by changing exciton dynamics [1]. Here, we present direct quantitative investigations of chemical p-doping by means of electron paramagnetic resonance (EPR), using a spin count reference sample. We estimated the p-doping concentrations on our SWNTs over a wide range, gaining new insight into the widely discussed topic of charge carrier confinement.

1. Eckstein et. al., Localized Charges Control Exciton Energetics and Energy-Dissipation in Doped Carbon Nanotubes, ACS Nano 2017, DOI:10.1021/acsnano.7b05543

CPP 77.9 Fri 12:00 C 243

Direct evidence of strong detrimental electronic interactions in solution processed doped organic semiconductors — •Ajay Jha[1], Hong-Guang Duan[1,2,3], Vandana Tiwari[1], Michael Thorwart[2,3], and R. J. Dwayne Miller[1,3,4] — [1]MPSD, Hamburg, Germany — [2]I. Institut für Theoretische Physik, UH, Germany — [3]CUI, Hamburg, Germany — [4]University of Tornoto, Canada

Understanding the inherent electronic structure the ion-pairs is essential to formulate a rational basis for charge mobilities in doped organic electronic circuits. Here we apply two-dimensional electronic spectroscopy to investigate the electronic dynamics of ion-pair in a solution of F4TCNQ-doped conducting polymer, PBTTT as a model system. The Coulombic interaction between cation and anion results in strong electronic coupling within the PBTTT+F4TCNQ- ion-pair which is manifested by the well-resolved off-diagonal peaks in 2D spectra envisaging the electronic connectivity among the ions. A theoretical model which simulates the experimental data reveals that the electronic coupling strength of 250 cm-1 with an intermolecular distance of 4.5 Å between the ions. Our experiments in combination with the theoretical modeling capture the molecular details of the ion-pair which should pave the way towards rational tailoring of the ion-pairs in solution.

CPP 77.10 Fri 12:15 C 243

The density of states of n-doped organic thin films from simulations and experiments — Christopher Gaul[1], Sebastian Hutsch[1], Martin Schwarze[2], Sebastian Schellhammer[1], Fabio Bussolotti[3], Satoshi Kera[3], Gianaurelio Cuniberti[1], Karl Leo[2], and •Frank Ortmann[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, Germany — [2]Dresden Integrated Center for Applied Physics and Photonic Materials, TU Dresden, Germany — [3]Institute for Molecular Science, Okasaki, Japan

Doping plays a crucial role in semiconductor physics where n-doping is controlled by the ionisation energy of the impurity relative to the conduction band edge. In organic semiconductors, efficient doping may be dominated by different effects, which are presently not well understood. Here, we study n-doping of C60 as prototypical material by simulating the density of states of the doped system in the density functional theory framework. We simulate the Fermi level position which compares well with experimental results from direct and inverse photoemission spectroscopy. From these results, we extract relevant factors that influence the doping efficiency.

CPP 77.11 Fri 12:30 C 243

State of matter dependent charge transfer interactions between planar molecules for doping applications — •Andreas Opitz[1], Paul Beyer[1], Duc Pham[1], Clea Peter[1], Norbert Koch[1,2], Dmitrii Nabok[1], Claudia Draxl[1], Lutz Grubert[1], Stefan Hecht[1], and Caterina Cocchi[1] — [1]Humboldt-Universität zu Berlin, Germany — [2]Helmholtz-Zentrum Berlin, Germany

Controlling the electrical conductivity of organic semiconductors is a key requirement for organic electronics, nowadays realized mostly by molecular dopants. Two doping mechanisms, i.e., charge transfer complex (CTC) and ion pair (IPA) formation, have been reported, but their occurrence depending on molecular structure, energy levels, and structure of thin films is elusive. Here, we study the p-type doping of the planar molecule dibenzo-tetrathiafulvalene (DBTTF) as semiconductor, with the planar electron acceptors tetracyano-naphthoquinodimethane (TCNNQ) and hexafluoro-TCNNQ (F6TCNNQ) as dopants. The conductivity increase is stronger for F6TCNNQ than for TCNNQ. Optical spectroscopy reveals the presence of CTCs for DBTTF:TCNNQ blends and CTC and IPA formation for DBTTF:F6TCNNQ blends. We discuss the different fundamental semiconductor-dopant interactions in solution and in solid-state with the aid of energy levels measurements, many-body perturbation theory calculations, absorption and vibrational spectroscopy. The presence of both charge transfer mechanisms in this set of compounds gives us access to their doping efficiency, which is higher for IPA than for CTC formation.

CPP 77.12 Fri 12:45 C 243

Photoinduced Charge Carrier Transport at (001) Pentacene/Perfluoropentacene Crystal Interfaces — •Sebastian Hammer[1] and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Mixed Pentacene:Perfluoropentacene (P:PFP) thin films have been reported archetypical donor-acceptor heterojunctions for examining the optical characteristics of charge transfer states [1]. However, aiming for possible effects on charge carrier transport at P/PFP interfaces, thin film boundaries impose severe limitations and thus, require the examination of photoinduced effects on the interface conductivity by means of well-defined crystal surfaces. For this purpose, pentacene single crystals were grown by horizontal physical vapor deposition with the (001) orientation of the crystal surface being confirmed by X-ray diffraction. PFP layers of various thicknesses between 5 to 50 nm were evaporated on top of the (001) surface and their morphology was analyzed by complementary AFM and XRD measurements. Illuminating the (001) P/PFP interface with a 532 nm cw-laser we observed a pronounced increase of the interface conductivity by up to 50% with respect to the neat pentacene crystal depending on the PFP top layer thickness as well as on the electric field applied. Utilizing different illumination geometries and temperature dependent measurements we will discuss the origin of the conductivity increase and its relation to charge transfer states and injection effects.

[1] Anger, F., et. al., *JCP* **136**, 054701 (2012)

CPP 78: Hybrid and Perovskite Photovoltaics II

Time: Friday 9:30–12:45 Location: C 264

CPP 78.1 Fri 9:30 C 264

Trap State Dynamics and Phase Transition in MAPbI3 — Tobias Seewald, Carola Ebenhoch, Susanne Birkhold, and •Lukas Schmidt-Mende — University of Konstanz

Perovskite semiconductors are a new class of semiconductors, significantly different from organic and also inorganic semiconductors. For efficient charge carrier gtobiaseneration, it is essential to minimize non-radiative recombination that can be initiated by energetic trap states. For this purpose, we have studied polycrystalline methylammonium lead iodide perovskite films with varying crystal sizes. Morphology and crystallinity have been modified by means of methylamine gas induced defect healing. Time-resolved photoluminescence as well as pump-probe spectroscopy have been applied in order to relate trap state distribution with crystal sizes and grain boundaries. In this study we can demonstrate the importance of large crystal grains, which allow high carrier mobilities and reduced non-radiative losses that are crucial for efficient solar cell devices. Furthermore, we have investigated the mechanism of the orthorhombic to tetragonal phase transition in MAPbI3 and the resulting changes in material properties. We present experimental evidence for a transient intermediate phase in MAPbI3 that occurs prior to the phase transition into the tetragonal phase, which might be induced by an increasing liberation/polarization of the organic cation within the orthorhombic phase at low temperatures. Our results demonstrate that this phase transition has strong impact on solar cell performance parameters.

CPP 78.2 Fri 9:45 C 264

Characterization and phase identification in cesium lead bromide thin films by correlative scanning electron microscopy — •Sebastián Caicedo-Dávila[1], Hannah Funk[1], Christian Müller[2], Michael Sendner[3], Robert Lovrincic[2], and Daniel Abou-Ras[1] — [1]Helmholtz Zentrum Berlin for Materials and Energy, Berlin, Germany — [2]Institute for High-Frequency Technology, InnovationLab, TU Braunschweig, Heidelberg, Germany — [3]Kirchhoff Institute of Physics, Heidelberg University, Heidelberg, Germany

Designing high-efficiency solar cells based on wide-gap, halide-perovskite absorbers is challenging, and understanding what limits the performance of such devices is still an open issue in the field. One of the wide-gap materials of interest is cesium lead bromide. If deposited as thin film, various Cs-Pb-Br phases may be present. Identification of these phases, their distribution at a microscopic level, as well as the correlation between microscopic, optoelectronic properties with macroscopic materials characteristics are fundamental tasks in research and development. In the present contribution, we report on local compositions and optoelectronic properties of Cs-Pb-Br thin films synthesized by spin-coating and coevaporation, which were analyzed by using SEM imaging, energy-dispersive X-ray spectrometry, cathodoluminescence, XRD, and photoluminescence spectroscopy. We discuss the different phase distribution and its dependence on synthesis method, and microscopic structuring of the film, the challenges concerning specimen preparation for more advanced SEM techniques, and the issue of damaging the sample by the electron beam.

CPP 78.3 Fri 10:00 C 264

Ingression of Moisture into Hybrid Perovskite Thin Films Probed with In-Situ GISANS — •Johannes Schlipf[1], Lorenz Biessmann[1], Lukas Oesinghaus[2], Ezzeldin Metwalli[1], Lionel Porcar[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]TU München, Physik-Department and ZNN, LS Physics of Synthetic Biological Systems, 85748 Garching — [3]Institut Laue-Langevin, 38042 Grenoble, France

Solution-processed hybrid perovskites are of great interest for photovoltaics. However, polycrystalline perovskite thin films show strong degradation in humid atmosphere which poses an important challenge for large-scale market introduction. With in-situ grazing incidence neutron scattering (GISANS) we analyze water content, degradation products and morphological changes during prolonged exposure to several humidity levels. At the highest humidity levels, formation of metastable hydrate phases is accompanied by domain swelling and transforms the facetted crystals to a pebble-like form. The films incorporate much more water than can be integrated in the hydrates. In low ambient humidity, around 10 vol% of water is adsorbed on the crystals without formation of crystalline degradation products. Thus, although production in ambient atmosphere is of interest for industrial production it might lead to long-term degradation without appropriate countermeasures.

CPP 78.4 Fri 10:15 C 264

Exciton-dominated core-level absorption spectra of hybrid organic-inorganic lead halide perovskites — •Christian Vorwerk[1,2], Claudia Hartmann[3], Caterina Cocchi[1,2], Golnaz Sadoughi[4], Severin Habisreutinger[4], Roberto Félix[3], Regan Wilks[3,5], Henry Snaith[4], Marcus Bär[3,5], and Claudia Draxl[1,2] — [1]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]European Theoretical Spectroscopy Facility — [3]Renewable Energy, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany — [4]Clarendon Laboratory, Department of Physics, University of Oxford, Oxford OX1 3PU, United Kingdom — [5]Energy Materials In-Situ Laboratory Berlin (EMIL), Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany

In a combined theoretical and experimental work, we investigate x-ray absorption near-edge spectra (XANES) from the iodine L_3 and the lead M_5 edge of the methyl-ammonium lead iodide (MAPbI$_3$) hybrid inorganic-organic perovskite and its binary phase PbI$_2$. We find that the absorption onsets are dominated by bound excitons with sizable binding energies of a few hundred meV and pronounced anisotropy. The spectra of both materials exhibit remarkable similarities, suggesting that the fingerprints of core excitations in MAPbI$_3$ are essentially given by its inorganic component, with negligible influence from the organic groups. Our theoretical analysis allows for an insightful characterization of experimental observations in this complex material.

CPP 78.5 Fri 10:30 C 264

Assessing density functionals using many body theory for hybrid perovskites — •Menno Bokdam, Jonathan Lahnsteiner, Benjamin Ramberger, Tobias Schäfer, and Georg Kresse — University of Vienna, Faculty of Physics and Center for Computational Materials Sciences, Vienna, Austria

Which density functional is the "best" for structure simulations of a particular material? A concise, first principles, approach to answer this question is presented. The random phase approximation (RPA)— an accurate many body theory— is used to evaluate various density functionals.[1] To demonstrate and verify the method, we apply it to the hybrid perovskite MAPbI$_3$, a promising new solar cell material. The evaluation is done by first creating finite temperature ensembles for small supercells using RPA molecular dynamics, and then evaluating the variance between the RPA and various approximate density functionals for these ensembles. We find that, contrary to recent suggestions, van der Waals functionals do not improve the description of the material, whereas hybrid functionals and the SCAN (strongly constrained appropriately normed) density functional yield very good agreement with the RPA. Finally, our study shows that in the room temperature tetragonal phase of MAPbI$_3$, the molecules are preferentially parallel to the shorter lattice vectors but reorientation on ps time scales is still possible.

[1] Bokdam et. al., Phys. Rev. Lett. 119, 145501 (2017)

CPP 78.6 Fri 10:45 C 264

The Finite Temperature Structure of the MAPbI3 Perovskite: Comparing Exchange-Correlation Potentials, Force Fields and Model Hamiltonians — •Jonathan Lahnsteiner[1], Georg Kresse[1], Jurn Heinen[2], and Menno Bokdam[1] — [1]University of Vienna, Faculty of Physics and Center of Computational Materials Science, Vienna Austria — [2]Van 't Hoff Institute for Molecular Sciences, University of Amsterdam

Determining the finite temperature structure of the hybrid perovskite MAPbI$_3$ at high accuracy is a challenge for both experimental and theoretical methods. A very powerful computational method is *ab-initio* molecular dynamics. It comes with the necessity of choosing a density functional approximation which directly influences the atomic structure. The complexity of the system has lead to the development of more approximate methods, such as classical force fields and model hamiltonians. Here we compare the different computational methods by analysis of the MA molecular ordering patterns in one consistent manor. For those methods that also describe the PbI$_3$ framework its symmetry is analyzed. Available experimental data in literature is discussed and compared to the outcomes of the different methods. The spread in these data is still too large to uniquely determine a method that 'best' describes the perovskite. However, the comparison on equal footing between the computational methods does allow to evaluate the applicability of the different approximations.

15 min. break

CPP 78.7 Fri 11:15 C 264

Role of Förster Resonance Energy Transfer for Efficient Charge Generation at Hybrid Heterointerfaces — •Stefan Schupp, Philipp Ehrenreich, and Lukas Schmidt-Mende — Department of Physics, University of Konstanz, Universitätsstraße 10, 78457 Konstanz, Germany

During the last two decades, tremendous progress was made in the development of efficient dye-sensitized solar cells with power conversion efficiencies of more than 10%. In this context, performance improvements are commonly related with chemical engineering, i.e. the design of new chemical compounds with optimized absorption characteristics. So far, transparent hole transporting layers are used although polymers offer the conceptual advantage to act not only as hole transporting materials but also as an additional photoactive layer. In a recent study, we have demonstrated that Förster resonance energy transfer (FRET) is a promising strategy to enhance photocurrent contributions from the polymer, while loss channels have stayed unclear. In this contribution, we will generalize our findings and offer new design rules, which help to engineer highly efficient hybrid polymer-metal oxide interfaces. By a comparison of eight different dye-polymer combinations, we tune the FRET efficiency and energy landscape at the interface systematically. This combined analysis helps to understand fundamental loss channels of hybrid heterostructures and offers strategies to bring hybrid solar cells on a competitive level.

CPP 78.8 Fri 11:30 C 264

LASER PATTERNING OF PEROVSKITE SOLAR CELLS FOR MINI-MODULE FABRICATION — •Christof Schultz[1], Felix Schneider[1,2], Marko Jost[3], Lukas Kegelmann[3], Andreas Bartelt[1], Bernd Rech[4], Rutger Schlatmann[1,2], Steve Albrecht[3], and Bert Stegemann[1] — [1]HTW Berlin - University of Applied Sciences, Wilhelminenhofstr. 75A, D-12459 Berlin — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, PVcomB, Schwarzschildstr. 3, D-12489 Berlin — [3]Helmholtz-Zentrum Berlin, Nachwuchsgruppe Perowskit Tandemsolarzellen, Kekuléstraße 5, D-12489 Berlin — [4]Helmholtz-Zentrum Berlin, Institut für Silizium-Photovoltaik, Kekuléstraße 5, 12489 Berlin

Metal halide perovskite (MHP) solar cells have been rapidly improved over the last years. Successful up-scaling from lab-scales to large module sizes requires monolithical interconnection processes. Here we report on laser scribing processes of the P1, P2 and P3 patterning steps to interconnect perovskite solar cells for module fabrication. Particular emphasis is put on the P2 laser patterning step as it is known to induce detrimental material modifications of the absorber layer mostly at the bottom and in the vicinity of the scribed lines. By systematic variation of the pulse length (ns, ps), the wavelength (1064 / 532 / 355 nm) and the processing side (glass-/ layer-side) suitable process windows were established and optimized. Based on systematic analysis of the laser-matter interaction the selective layer removal, the proper morphology and the electrical functionality were elucidated allowing successful fabrication of a mini-module.

CPP 78.9 Fri 11:45 C 264

In situ study of degradation in P3HT-titania based solid-state dye-sensitized solar cells — •Lin Song[1], Weijia Wang[1], Stephan Pröller[2], Daniel Moseguí González[1], Johannes Schlipf[1], Christoph J. Schaffer[1], Kristina Peters[3], Eva M. Herzig[2], Sigrid Bernstorff[4], Thomas Bein[3], Dina Fattakhova-Rohlfing[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]TU München, MSE, Herzig Group, 85748 Garching — [3]LMU München, Department of Chemistry and CENS, 81377 München — [4]Elettra-Sincrotrone Trieste 34149 Trieste, Italy

Solid state dye sensitized solar cells (ssDSSCs) have received great attention over last decades due to low costs, ease of production and high efficiencies. However, the stability of these devices is still not verified. To address this issue, the degradation of ssDSSCs is studied in the present work. To make a comparison, mesoporous titania films with different pore size are used as photoanodes. The impact of pore size on temporal evolution of the P3HT crystallites under continuous solar illumination is compared using in situ grazing-incidence wide-angle x-ray scattering (GIWAXS) measurements, and the development of the photovoltaic characteristics is probed in parallel [1]. The findings of the in-situ study show that pore size plays an important role in the device performance and stability.

[1] ACS Energy Lett.2, 991-997 (2017)

CPP 78.10 Fri 12:00 C 264

Increased Photovoltage by Use of Metal Complexes as Redox Couples in Dye-Sensitized Solar Cells based on Low-Temperature Electrodeposited ZnO — •Raffael Ruess, Thi Hai Quyen Nguyen, Sebastian Haas, Andreas Ringleb, and Derck Schlettwein — IAP, JLU Giessen, Germany

Dye-sensitized solar cells (DSSCs) have received continued interest because of new record efficiencies (up to 14.3 %) and low energy payback times. This work is focused on DSSCs based on electrodeposited, porous ZnO which allows low preparation temperatures to further reduce energy consumption of cell production and to use various kinds of substrates such as flexible foils, threads, wires or fibers. One of the most promising strategies to reduce voltage losses in the cells consists in replacement of the I^-/I_3^- redox electrolyte by metal complex redox couples that show fast electron transfer kinetics at low driving force. Detailed photoelectrochemical studies are used to investigate charge transfer and transport in complete photovoltaic devices. Recombination at the ZnO/electrolyte interface as well as mass transport in the electrolyte have been identified as performance-limiting factors. Control of these factors was achieved by manipulating the electrolyte composition leading to promising power conversion efficiencies of 3.56 % or 3.85 % with cobalt-based or copper-based redox couples. This work shows that such metal complex redox couples can also be applied in cells based on ZnO and opens the door for further improvements in device efficiency of this type of DSSCs.

CPP 78.11 Fri 12:15 C 264

macro- and nano-scale morphology evolution during in situ spray coating of titania films for perovskite solar cells — •Bo Su[1], Herbert A. Caller-Guzman[1], Volker Körstgens[1], Yichuan Rui[2], Yuan Yao[1], Nitin Saxena[1], Gonzalo Santoro[3], Stephan V. Roth[3], and Peter Müller-Buschbaum[1] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, 85748 Garching — [2]College of Chemistry and Chemical Engineering, Shanghai University of Engineering Science, Shanghai 201620, China — [3]DESY, 22607 Hamburg

To scale-up deposition processes, the use of spray deposition is advantageous, because it is easy to be controled and has no limitation concerning substrate geometry. In this study, the structure evolution of mesoporous titania films, with a controllable pore size, is characterized by in situ grazing incidence small angle X-ray scattering (GISAXS) during the spray process. For the applied spray conditions, we observe micelle deposition, evaporation of the solvent and transformation of the morphology towards equilibrium. All processes influence the structure features on the nano-scale. On the macro-scale, the kinetics and thermodynamics of the spray depositions processes are simulated. We find a good agreement with the large-scale morphology of the spray-coated films obtained in the experiments. Hybrid perovskite (methylammonium lead iodide) solar cells based on the sprayed titania film are fabricated as a showcase of the developed spray-deposition for solar cell applications.

CPP 78.12 Fri 12:30 C 264

Investigation of mobility controlled amphiphilic diblock copolymer templating for hybrid photovoltaic applications — •Nuri Hohn[1], Steffen Schlosser[1], Lorenz Biessmann[1], Sebastian Grott[1], Senlin Xia[1], Kun Wang[1], Matthias Schwartzkopf[2], Stephan Roth[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]DESY, 22607 Hamburg — [3]KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Schweden

Current research in the field of hybrid photovoltaics aims to develop devices, which benefit from the advantages of both their organic and inorganic nature. While the organic part can contribute flexibility, potential low cost and possible large scale production, the inorganic counterpart offers chemical and physical stability. Nevertheless, one major issue in device fabrication still consists of the backfilling process. Therefore, tuning of the pore size of the inorganic thin films is of importance. Based on an amphiphilic diblock copolymer templating with polystyrene-b-polyethylene oxide and tuning of the dryness state of the casting solution different morphologies are achieved after blade coating. The introduced method is expected to facilitate the optimization process of high surface-to-volume ratio against sufficiently large pores for efficient backfilling. Surface and bulk analysis is carried out via SEM and grazing incidence small angle X-ray scattering.

CPP 79: Wetting, Microfluidics and Confined Liquids II

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

CPP 79.1 Fri 9:30 PC 203

Water Mobility in the Interfacial Quasi-Liquid Layer of Ice/Clay Nanocomposites — •Markus Mezger[1,2], Hailong Li[2], Julian Mars[1,2], Henning Weiss[2], and Wiebke Lohstroh[3] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz — [2]Max-Planck-Institut für Polymerforschung, Mainz — [3]Heinz Maier-Leibnitz Zentrum, Garching

At solid/ice interfaces, a quasi-liquid premelting layer is formed at temperatures below the melting point of bulk water. The water mobility within this premelting layer in ice/clay nanocomposites was determined by quasi elastic neutron scattering. Connections between the translational diffusion coefficient D_t and the surface properties were studied for three clays, serving as model systems for permafrost. Below the bulk melting point, a rapid decrease of D_t is found for all systems, reaching plateau values below $-4\,^\circ\mathrm{C}$. At this temperature, D_t in the premelting layer is reduced up to a factor of two compared to super cooled bulk water. Adjacent to charged vermiculite the lowest water mobility was observed, followed by kaolin and the more hydrophobic talc.

CPP 79.2 Fri 9:45 PC 203

Dynamic activity of water confined in hydrophobic and hydrophilic pores probed by neutron spectroscopy — •Margarita Russina[1], Veronika Grzimek[1], Moritz-Casper Schlegel[1,2], and Anita Petrova[1,3] — [1]Helmholtz Zentrum Berlin für Materialied und Energie, Hahn-Meitner Platz 1, 14109 Berlin — [2]BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin , Germany — [3]Saint-Petersburg State University , Faculty of Physics, Petrodvorets, Ulyanovskaya str., 1, Saint-Petersburg, Russia, 198504

The understanding of hydrogen bonds formation in various environment and criteria governing the molecular mobility at nanoscale is of high importance to various fields of applications. Using neutron spectroscopy as a powerful nanoscope we have investigated molecular dynamics of water in hydrophobic and hydrophilic nanoconfinement in a very broad temperature range of 20-300 K. By an aimed selection of the confining systems we were able to follow the molecular behavior in pores of various sizes and in environments with variable degrees of water - host interactions. Changing the amount of confined water allowed us an additional systematic insight. Thus, in hydrophobic zeolite AlPO4-5 we have found pronounced adsorption induced structural contraction as a result of guest-host interactions. Furthermore, with the evolution of the growing water network and increasing guest-guest interactions we observe non-linear changes of the mean square displacement, experimentally determined on the picosecond time scale.

CPP 79.3 Fri 10:00 PC 203

Structure and Dynamics of Confined Liquids Studied by an X-ray Surface Force Apparatus — •Henning Weiss[1], Hsiu-Wei Cheng[2], Julian Mars[1,3], Claudia Merola[2], Veijo Honkimäki[4], Markus Valtiner[2], and Markus Mezger[1,3] — [1]Max Planck Institut for Polymer Research, Mainz, Germany — [2]TU Wien, Institute for Applied Physics, Wien, Austria — [3]Johannes Gutenberg University Mainz, Institute of Physics, Mainz, Germany — [4]ESRF-The European Synchrotron, Grenoble, France

Structure and dynamics of confined liquids were probed by an in-situ X-ray surface force apparatus in plane-cylinder geometry. Our novel device can shear and compress/decompress soft matter within a precisely controlled slit pore confinement. Complementary structural information is obtained by X-ray scattering and simultaneous force measurements. Here, we present results on the structural relaxation of confined liquid crystals (LCs) as reaction to external stimuli. For the smectic LC 8CB we investigated defect-formation and relaxation processes during subsequent compression and decompression cycles. In the second example, an 80 nm thin film of the wet ionic liquid $[\mathrm{C_{10}mim}]^+$ $[\mathrm{Cl}]^-$ in the columnar LC phase was sheared. The observed mesoscopic orientation induced by oscillatory shear is explained by the anisotropic mobility of the mesogens.

CPP 79.4 Fri 10:15 PC 203

Influence of the ordering of depletants on structural forces in thin liquid films — •Michael Ludwig[1], Sebastian Schön[2], and Regine von Klitzing[1] — [1]Technische Universität Darmstadt — [2]Technische Universität Berlin

Structural forces are observed when pure solvents and ionic liquids, as well as dispersions containing nanoparticles, micelles, polymers or polyelectrolytes are confined between two smooth surfaces. Upon surface-approach, liquid matter has to be depleted from the vicinity of the surfaces, altering the interactions between the surfaces.

Recent experimental studies reveal the superposition of structural forces with DLVO-type forces [1,2]. Here, we will focus on nanoparticle dispersions in confinement between two charged silica-surfaces, as probed in our experiments using a colloidal-probe atomic force microscope (CP-AFM). An additional repulsive term has to be introduced to accurately fit experimental data. This additional term will be discussed in terms of the DLVO-framework.

At high concentrations of depletants, structural force profiles appear to show oscillatory behaviour. The corresponding wavelength λ correlates with the mean particle distance of the depleting particles in the bulk liquid [3]. Different dependencies between wavelength λ and particle number density ρ will be presented considering the bulk liquid geometries.

[1] S. Perkin et al., Phys. Rev. Lett. 119, 026002 (2017) [2] G. Trefalt et al., Phys. Rev. Lett. 177, 088001 (2016) [3] R. von Klitzing et al., Soft Matter 7, 10899 (2011)

CPP 79.5 Fri 10:30 PC 203

Non-equilibrium surface critical dynamics in a confined binary liquid mixture — •Sutapa Roy[1], Felix Höfling[2], and Siegfried Dietrich[1] — [1]Max-Planck-Institute for Intelligent Systems, Stuttgart, Germany and Institute for Theoretical Physics IV, University of Stuttgart, Germany — [2]Freie Universität Berlin, Department of Mathematics and Computer Science, Berlin, Germany

Close to a solid surface the static and dynamic properties of a fluid deviate significantly from their bulk behaviour. In this context, by using molecular dynamics simulations, we investigate the rich non-equilibrium relaxation dynamics of a binary liquid mixture [1] confined to a slit pore, fully respecting hydrodynamic conservation laws. A sudden temperature quench of the liquid from the disordered phase to its bulk demixing critical point yields a non-equilibrium response. The corresponding dynamics, characterised by the two-time auto-correlator of the position-dependent order parameter, exhibits aging and scaling [2]. Analysis of the aging behaviour allows us to quantify the crossover from surface- to bulk-like dynamics. Our results for the surface adsorption profiles in equilibrium are compared with recent theoretical predictions for the canonical ensemble [3]. To the best of our knowledge, this study is the first one to explore both surface and bulk *aging* phenomena of a liquid at criticality.

[1] S. Roy, S. Dietrich & F. Höfling, J. Chem. Phys. **145** 134505 (2016). [2] S. Roy, F. Höfling & S. Dietrich, unpublished (2017). [3] M. Gross, O. Vasilyev, A. Gambassi & S. Dietrich, Phys. Rev. E **94** 022103 (2016).

CPP 79.6 Fri 10:45 PC 203

Electrolyte solutions confined by non-uniform walls — •Maximilian Mussotter and Markus Bier — Max-Planck Institut für Intelligente Systeme und Universität Stuttgart, 70569 Stuttgart, Germany

In contrast to fluids comprising electrically neutral constituents and uncharged walls, the widely used assumption of substrates with uniform wall-fluid interactions is questionable beyond molecular length scales in the context of charged substrates and dilute electrolyte solutions, where the influence of non-uniformities can be on the scale of the Debye length. For this reason the goal of this work was to deepen understanding of electrolyte solutions in contact with non-uniformly charged substrates. The system is studied by means of classical density functional theory, within the framework of square-gradient and double-parabola approximation. This work is intended to lay the foundations for future studies of fluids confined by non-uniform boundaries.

CPP 79.7 Fri 11:00 PC 203

Metadynamics calculation of chemical potential in dense and confined fluids — •Claudio Perego[1] and Michele Parrinello[2] — [1]Max Planck Institute for Polymer Research, Mainz (De) — [2]Swiss Federal Institute of Technology, Zurich (Ch)

Chemical potential is a crucial thermodynamic quantity, regulating phase and chemical equilibria in a wide range of systems. The calculation of chemical potential in dense fluids represents a long-standing challenge in molecular simulations. An established approach builds on Widom's method, in which chemical potential is computed by sampling the insertion energy of a test particle. The resulting value is mostly determined by low energy insertions, in which the test particle is placed in a proper cavity within the system particles. In dense liquids such cavities are rarely available, and the sampling is restricted to large insertion energies, preventing the convergence of the estimate. Here we present a new method for computing the chemical potential in dense liquids. The technique builds on metadynamics to extend the insertion energies to the relevant low energy region, inaccessible in unbiased simulations. We show that the method can be also generalized for the computation of chemical potential in non-homogeneous fluids, which represents a crucial step for the study of nano-fluidics and confined liquids. The technique is then tested with both homogeneous and non-homogeneous Lennard-Jones fluids. As a result accurate chemical potential estimates are obtained even at large densities, where the classical approach fails.

CPP 79.8 Fri 11:15 PC 203

Heisenberg fluids under confinement — •Stefanie Maria Wandrei[1], Roland Roth[2], and Martin Schoen[1] — [1]Technische Universität Berlin — [2]Eberhard Karls Universität Tübingen

In this work we employ classical density functional theory (DFT) to investigate the behavior of a Heisenberg fluid at a single wall or confined to a nanoscopic slit pore of variable width. We consider three different types of confining surfaces: hard walls, simple attractive walls, and attractive walls with an additional field acting on the spins. To account for the locality of the density we use the White Bear version of fundamental measure theory. This allows us to investigate in greater detail than in previous works the effect that competing external fields have on the behavior of the confined fluid.

CPP 80: Organic Thin Films, Organic-Inorganic Interfaces: Session II (joint session DS/CPP)

Time: Friday 9:30–11:00 Location: H 0111

CPP 80.1 Fri 9:30 H 0111

Infrared studies of device relevant organic/inorganic interfaces: energetic and morphological insights — •Sabina Hillebrandt[1,2], Sebastian Beck[1,2], and Annemarie Pucci[1,2] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Germany — [2]InnovationLab, Heidelberg, Germany

Organic electronic devices consist of stacked layers as well as inorganic materials. The device performance is mainly influenced by the interfaces of these layers. The investigation of charge generation, injection, and transport at these interfaces is a major key to the basic understanding of the fundamental mechanisms in organic electronics. We use self-assembled monolayers (SAM) in this context to engineer the surface of certain electrode materials, e.g. indium tin oxide (ITO) and metal surfaces, in order to improve charge injection at the organic/inorganic interface. With their inherent dipole SAMs are ought to improve the energetic alignment at the interface as well as to change the surface energy and thus the contact angle. Infrared (IR) spectroscopic studies supported by density functional theory (DFT) calculations reveal in addition to the molecular orientation of such SAMs the influence on that orientation on the subsequent organic semiconductor material. Furthermore, energy transfer between the electrode material and its modification and the organic semiconductor can be investigated, giving a deep insight into the energetic and morphological interplay at the interface.

CPP 80.2 Fri 9:45 H 0111

Probing the orientation of phosphorescent Iridium complexes by impedance spectroscopy — •Markus Schmid, Thomas Lampe, Alexander Hofmann, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Impedance spectroscopy (IS) is a powerful, non-destructive method to analyze organic semiconductors and their interfaces. In organic bilayer devices, that contain one polar material, IS can be used to measure the interfacial charge density between the two semiconductors. This polarization results from partially aligned permanent dipole moments. If the permanent molecular dipole moment is known, conclusions about the molecular orientation are possible [1].

In this study we present results from IS for different polar Iridium complexes that are commonly used as emitters in organic light emitting diodes. By calculating their permanent dipole moment and their transition dipole moment via density functional theory we relate the average orientation of both vectors in the film. Additionally, the measured alignment of the molecules is compared to molecular dynamic simulations. We find good agreement between both, the often studied orientation of the transition dipole moment and the simulations.

[1] Jäger, Lars, *et. al.* AIP Advances **6**, 095220 (2016)

CPP 80.3 Fri 10:00 H 0111

Comparative in-situ studies of Au sputter growth on homo and di-block co-polymer — •Pallavi Pandit[1], Matthias Schwartzkopf[1], Andre Rothkirch[1], Bjoern Fricke[1], Marc Gensch[1], Alexander Hinz[2], Oleksandr Polonskyi[2], Thomas Strunskus[2], Simon Schaper[3], Franziska C. Löhrer[3], Volker Körstgens[3], Franz Faupel[2], Peter Müller-Buschbaum[3], and Stephan V. Roth[1,4] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]CAU zu Kiel, LS Materialverbunde, 24143 Kiel — [3]Physik-Department, LS Funktionelle Materialien, 85748 Garching — [4]KTH, Teknikringen 56-58, SE-100 44 Stockholm

Nanostructured gold (Au) attracts great technological interest and it is a promising candidate for functional, optical and electronic applications. A tailored metal nanoparticle-polymer interface improves the functionality of the system; attributed to the polymer-metal interactions, which are dominated by their interfacial interactions. Sputter deposition technique has been used for depositing metallic layer of few nanometer thicknesses in a controlled fashion on polymer surfaces [1]. To this end, we have investigated the morphological changes occurring at the metal-polymer interface during deposition using GISAXS and GIWAXS [2]. Optical properties of the system have also been studied in-situ and are correlated with the morphological properties of the gold nanocluster on polystyrene, polymethelmethacrlate and the corresponding di-block co-polymer. [1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 9, 5629 (2017). [2] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015).

CPP 80.4 Fri 10:15 H 0111

Graphene based biosensing surfaces studied by IR-nanopolarimetry — •Karsten Hinrichs[1], Timur Shaykhutdinov[1], Christoph Kratz[1], Felix Rösicke[2], Cristoph Arenz[3], Norbert H. Nickel[2], and Jörg Rappich[2] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Schwarzschildstr 8, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekuléstr. 5, 12489, Berlin, Germany — [3]Institut für Chemie der Humboldt-Universität zu Berlin. Brook-Taylor-Str. 2, 12489 Berlin, Germany

AFM-IR based nanopolarimetry [1] for analysis of large area graphene pre-functionalized by diazonium compounds [2] and recognition of cysteine-modified peptide nucleic acid (PNA) [3] is presented. Homogeneity of the biosensing surfaces and the secondary structure of the PNA was studied by AFM-IR measurements. AFM-IR in a sensitive modus with synchronization between the pulse rate of the quantum cascade laser used as IR light source and the resonance of the cantilever can provide IR spectra in several seconds only. This facilitates direct insight into chemical composition, intermolecular interactions, and molecular orientation in nanoscale sub-ensembles.

[1] T. Shaykhutdinovet al, Supramolecular Orientation in Anisotropic Assemblies by IR Nanopolarimetry. ACS Macro Letters 2017, 598-602. [2] F. Rösicke et al, Chem. Commun. 53 (2017) 9308-9311. [3] K. Hinrichs et al, Encyclopedia of Interfacial Chemistry: Surface Science and Electrochemistry 2018.

CPP 80.5 Fri 10:30 H 0111

Study of reactive ion beam planarization process of a negative tone resist for smoothing aluminium mirrors — •Melanie Ulitschka, Jens Bauer, Frank Frost, and Thomas Arnold — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, 04318 Leipzig

Mirror optics are a key component for a wide range of optical systems in lithography, imaging, as well as aerospace industry. For such a specific field of applications lightweight, good machinable aluminum alloys are suitable since the reflection coefficient ranges from the UV to the IR spectral region with values well above 90%. The surface error topography after commonly manufacturing by single-point diamond turning meets the requirements for applications in the infrared spectral range. To use the aluminum mirrors in the shortwave visible and UV-spectral range one technological solution is the coating of the Al optics with a nickel-phosphorous layer and a metallization layer on top to realize ultra-smooth highly reflective surfaces. Further reduction of the surface roughness of aluminum optics and a simplification of this process chain is preferable.Ion beam planarization processes are a promising technology to transfer the ultra-smooth surface of a planarization layer into the underlying aluminum substrate. An equal etch rate for planarization layer and aluminum is the prerequisite for the transfer process. The contribution comprises investigations on the influence of different ion beam parameters on the chemical modification of the layer during the etch process, the effect of thermal pre-treatment of the planarization layer and the etch rate selectivity of layer and substrate.

CPP 80.6 Fri 10:45 H 0111

Structure-Dependent Emission of 1-(Pyridin-2-yl)-3-(quinolin-2-yl)imidazo[1,5-a]quinoline — •Georg Albrecht[1,3], Jasmin Martha Herr[2,3], Hisao Yanagi[3], Richard Göttlich[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, JLU Giessen, Germany — [2]Institute of Organic Chemistry, JLU Giessen, Germany — [3]Nara Institute of Science and Technology, Japan

1,3-disubstituted imidazo[1,5-a]pyridines are receiving increased interest for applications in material science, mainly regarding organic light emitting diodes (OLED). In this work we studied the related 1-(pyridin-2-yl)-3-(quinolin-2-yl)imidazo[1,5-a]quinoline (PCIC) as a new and oxidation-stable blue emitter. Thin films were prepared by physical vapor deposition onto quartz glass, single crystals were grown from solutions or by entrainer sublimation. Thin films and crystals were characterized by AFM, XRD, optical absorbance and mainly by steady-state and time-resolved emission and compared to results obtained in solution. Storage of the originally amorphous thin film samples revealed an interesting crystallization behaviour, which could be resolved by fluorescence microscopy and comparison to the results obtained at single-crystals. A clear trend of red-shifted emission was observed for different crystalline phases relative to amorphous samples, corresponding to the change in molecular arrangement.

CPP 81: Active Matter (joint session BP/CPP/DY)

Time: Friday 9:30–12:00 Location: H 1058

CPP 81.1 Fri 9:30 H 1058

Collective cell behavior - a phase field active polar gel model — •Axel Voigt, Simon Praetorius, and Dennis Wenzel — TU Dresden, Institut für Wissenschaftliches Rechnen

We consider a continuum model for collective cell movement. Each cell is modeled by a phase field active polar gel model and the cells interact via steric interactions. We provide a finite element implementation with a parallel efficiency in the number of cells. This is achieved by considering each cell on a different processor and various improvements to reduce the communication overhead to deal with the cell-cell interactions. We demonstrate results for up to 1.000 cells.

CPP 81.2 Fri 9:45 H 1058

Statistical physics and hydrodynamics of passive/active mixtures — •Raphaël Jeanneret[1], Arnold Mathijssen[2], and Marco Polin[3] — [1]IMEDEA-UIB, Esporles, Spain — [2]Stanford University, Stanford, US — [3]Warwick University, Coventry, UK

In this talk I will present a series of experimental and theoretical results regarding the dynamics of passive particles in liquid bath of active ones. The active particles act here, via the flows they generate, as localized and erratic sources of momentum for the passive beads leading to non-trivial dynamics. Beyond their exciting features for the physicist, active/passive systems are worth studying quantitatively for applications as diverse as the transport of passive entities in cells, biogenic mixing (i.e. mixing of the ocean by living creatures), virus infection, cargo transport (e.g. drug delivery) or self-assembly (e.g. via motility-induced phase separation). The model system I consider is composed of the motile micro-alga Chlamydomonas reinhardtii, a model organism at numerous levels, and polystyrene beads. I will first show that the effective diffusion of micron-sized beads embedded in homogeneous suspensions of algae is greatly enhanced compared to their thermal counterpart. I will then demonstrate how this coarse-grained dynamics can be understood from the near-field hydrodynamics of the swimming organisms via hydrodynamical entrainment events. Finally I will talk about recent results regarding systems of weakly Brownian colloids in spatially heterogeneous suspensions of algae and show how our findings can be used to induce the spontaneous demixing of the two kinds of particles.

CPP 81.3 Fri 10:00 H 1058

Got worms? Collective feeding in C. elegans — •Robert Endres, Linus Schumacher, Serena Ding, and Andre Brown — Imperial College, London, United Kingdom

Collective behaviour, a hallmark of complex living systems, is often studied in groups of large animals or small cells, but less at the mesoscopic scale. Here, we investigate the collective feeding of the nematode C. elegans, known for its easy genetic manipulation and stereotypic worm postures. In this system, small genetic perturbations can lead to strikingly different population-level behaviors. First, we quantified behavioral differences between the 'solitary' lab strain and a 'social' aggregating mutant strain, using fluorescence imaging and many-worm tracking to probe the dynamics inside aggregates. Second, to understand the mechanism of aggregation, we drew on concepts from motility-induced phase transitions and developed a minimal model. Finally, using this model, we investigated the potential benefits of collective feeding to explain the predominance of aggregating strains in the wild.

CPP 81.4 Fri 10:15 H 1058

A continuum model to study coordination of tissue growth — •Maryam Aliee, Damir Vurnek, Sara Kaliman, and Ana-Sunčana Smith — Cluster of Excellence: Engineering of Advanced Materials, Friedrich-Alexander-University of Erlangen-Nürnberg

Living organisms represent fascinating and precise structures. It is still a big challenge to understand the mechanisms though which cells interact with each other and the environment to form reproducible patterns. We analyze how tissue growth is controlled by cell properties putting together a theoretical model and quantitative analysis of experiments. We measure carefully growth properties of a single-layered epithelium, cultured MDCK cells. In these experiments a group of several cells grows to a bigger colony. We observe the density of cells increases and a bulk region with a high constant density is established in the center, surrounded by the edge where cell density decreases. Our results demonstrate a gradual transition from an early exponential growth to a non-linear regime when growth speed increases with colony size.

We develop a continuum model to take into account cell mechanics and growth to study dynamics of tissues. We consider balance of cell number and forces for viscoelastic materials modified by active terms coming from cell division and apoptosis. We solve the equations with analytical and numerical methods. Our results show establishment of bulk and edge regions independent of many details. We study how the dynamics of the colony is controlled by cell characteristics and their interactions with surroundings. Remarkably, our model reproduces the nontrivial properties of MDCK growth in different experiments.

CPP 81.5 Fri 10:30 H 1058

Synthetic reconstitution of beating cilia — •Isabella Guido, Smrithika Subramani, Christian Westendorf, and Eberhard Bodenschatz — Max Planck Institute for dynamics and self-organization, Göttingen, Germany

Cilia are microscopic hair-like structures that present a rhythmic waving or beating motion and are found on the surface of almost all mammalian cells and on the body of some protozoan organisms. They are used for fluid flow based transport (e.g. removal of pollutants in the trachea) or for the locomotion in viscous fluid environments.

In our work we aim to develop synthetic ciliated systems able to propel themselves or to move fluids across a fixed surface. For this purpose we employ a bottom-up approach for assembling a simple system made of few building blocks adapted from natural cilia, namely microtubules and motor proteins. Using Kinesin-1, a processive motor powered by ATP hydrolysis, we synthesized a system containing MT bundles that are free to move in all planes, deviating from the conventional gliding assay. By binding them to a surface using a suitable anchor system, we are able to observe the microtubules-motor protein system oscillations in a manner that closely mimics ciliary movement.

The issue that we are addressing in our experiments is: how simple is the simplest system that is able to beat?

CPP 81.6 Fri 10:45 H 1058

DNA in the cell nucleus is organized similar to an active microemulsion — •Lennart Hilbert[1,2,3], Yuko Sato[4], Hiroshi Kimura[4], Frank Jülicher[1,3,5], Alf Honigmann[2], Vasily Zaburdaev[1,3], and Nadine Vastenhouw[2] — [1]Center for Systems Biology Dresden — [2]Max Planck Institute of Molecular Cell Biology and Genetics — [3]Max Planck Institute for the Physics of Complex Systems — [4]Tokyo Institute of Technology — [5]Center for Advancing Electronics Dresden

Inside cell nuclei, DNA is stored in the form of chromatin. Chromatin is three-dimensionally organized in response to transcription of DNA into RNA. Here, we studied the mechanisms by which transcription organizes chromatin, using experiments in zebrafish embryonic cells and theory. We show that transcription establishes an interspersed pattern of mutually exclusive chromatin-rich domains and RNA-rich domains. Ongoing transcriptional activity stabilizes the interspersed domain pattern by establishing contacts between the RNA and transcribed parts of chromatin. We explain our observations with an active microemulsion model based on two macromolecular mechanisms: (i) RNA/RNA-binding protein complexes and chromatin undergo phase separation, while (ii) transcription tethers RNA/RNA-binding proteins to chromatin and thereby forms amphiphile particles that intersperse the phases. Thus, three-dimensional DNA organization in the cell nucleus is an example of an unconventional, active microemulsion, stabilized by a catalytically active amphiphile that produces one of the emulsified phases.

CPP 81.7 Fri 11:00 H 1058

Size increases produce coordination trade-offs in a simple multicellular animal near criticality — Mircea R. Davidescu[1], •Pawel Romanczuk[2,3], Thomas Gregor[4], Corina E. Tarnita[1], and Iain D. Couzin[5,6] — [1]Dept. of Ecology and Evol. Biology, Princeton University ,USA — [2]Institute for Theoretical Biology, Dept. of Biology, Humboldt Universität zu Berlin, Germany — [3]Bernstein Center for Computational Neuroscience, Berlin, Germany — [4]Joseph Henry Laboratories of Physics, Princeton University, USA — [5]Dept. of Collective Behavior, MPIORN, Konstanz, Germany — [6]Dept. of Biology, University of Konstanz, Germany

Based on theoretical arguments from statistical physics, it has been suggested that collective systems in biology should operate close to criticality in order to maximize their susceptibility to external signals [Mora & Bialek, J Stat Phys, 144, 2 (2011)]. Recently, this hypothesis received increased attention in the context of collective behavior in biology. However, it is still rather controversial and up to know most support for it comes from idealized mathematical models and few experimental systems. Here, we will discuss some recent experimental observations of Placozoa (*Trichoplax Adhaerens*), a simple multicellular animal effectively corresponding to a quasi two-dimensional cellular sheet. By combining experimental data with simple mathematical model of Placozoa motion as a collective system, we find that the observed dynamics are indeed consistent with the criticality hypothesis, but as a consequence these simple animals without a central nervous system have to face a fundamental size-coordination trade-off.

CPP 81.8 Fri 11:15 H 1058

Harnessing emergence in bacterial populations: From biological mixing to active mechanics — •Anupam Sengupta — Institute for Environmental Engineering, ETH Zurich, Switzerland — Physics and Materials Science Research Unit, University of Luxembourg

At the scale of a single cell, interactions between a bacterium and its micro-environment represent a complex biophysical interface between phenotypic states (free-living planktonic or surface-attached sessile state) and external cues. In this talk I will discuss two recent works where we use experiments and modeling to elucidate how bacterial phenotype cross-talks with immediate micro-environment, and harnesses the emergent physics for biological functions. In the first case, we will see how Chromatium okenii, a 10 μm long purple sulphur bacterium, is capable of mixing over a meter thick layer of water in the Swiss Alpine lake, Lago di Cadagno. By changing the local fluid density, C. okenii is able to trigger convection rolls, creating a sustained well-mixed nutrient layer within an otherwise stratified lake. In the second instance, we will examine emergent geometrical and mechanical properties of a bacterial colony growing on a soft substrate. We show that such an expanding colony self-organizes into a “mosaic” of micro-domains consisting of highly aligned cells, before emerging into an active nematodynamic system. Interestingly, phenotypic traits - motility in the first and growth-induced stresses in the latter - couple with local hydrodynamics, to elicit important ecological functions at scales that can be orders of magnitude higher than single cells.

CPP 81.9 Fri 11:30 H 1058

Hydrodynamic theory of aster positioning by motor proteins — •Andrej Vilfan — J. Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

In fertilized egg cells of certain species the male pronucleus is transported to the center of the cell by growing an asymmetric microtubule aster, which then serves as a track for motor proteins carrying vesicles towards the center. Because these vesicles experience a viscous drag in the surrounding cytoplasm, the motors exert the opposite force on the microtubules. The asymmetry of the aster then leads to a net pulling force towards the cell center. Yet hydrodynamic interactions make the understanding of the process difficult.

Here we discuss a coarse-grained approach where we describe the aster as a porous medium and the moving vesicles as sources of an active pressure gradient. In parallel, we use computational models to determine the parameters of the continuum model. For realistic parameters, we show that a significant proportion (10-20%) of the motor force is converted to a pressure gradient and contributes to aster centering. We conclude that vesicle transport in a viscous environment is a surprisingly efficient way of force generation.

CPP 81.10 Fri 11:45 H 1058

Active polymer models for the 3D organization of chromosomes — •Johannes Nuebler[1], Geoffrey Fudenberg[2], Maxim Imakaev[1], Nezar Abdennur[1], and Leonid Mirny[1] — [1]Institute for Medical Engineering and Science, Massachusetts Institute of Technology, Cambridge, MA 02139, USA — [2]University of California, San Francisco, Gladstone Institutes, San Francisco, CA 94158, USA

Eukaryotic chromatin is far from being a randomly arranged polymer in the cell nucleus. Rather, a high degree of spatial organization on various length scales is revealed by Hi-C and imaging techniques. We show that the organization on intermediate scales emerges from the interplay of two mechanisms, one active and one passive: first, on the scale of one million basepairs and below, active formation of growing chromatin loops emerges as a general organizational principle throughout the cell cycle. Second, a block-copolymer based phase separation explains chromatin compartmentalization on larger scales. Interestingly, these processes interact: only the interplay of loop extrusion and spatial segregation explains a large number of experimental perturbations, namely removal of the loop extruder cohesin, removal of the cohesin boundary element CTCF and removal of the cohesin unloader Wapl, and it makes specific predictions for variations in the compartmental interaction and topological constraints (bioRxiv: https://doi.org/10.1101/196261).

CPP 82: Membranes and Vesicles II (joint session BP/CPP)

Time: Friday 9:30–12:00 Location: H 2013

CPP 82.1 Fri 9:30 H 2013

Change of thermodynamic state of cell membrane during an action potential — •Simon Fabiunke, Christian Fillafer, and Matthias Schneider — Medizinische und Biologische Physik, TU-Dortmund

Nonlinear pulses like action potential are considered to be purely electrical phenomena. However, it has been shown that thermal, mechanical, chemical and optical changes also occur at the excitable membrane. From a thermodynamic perspective such pulses have been described as a propagating state change in the cell membrane.

In the present work, we investigated the emission properties of a commonly used potential-sensitive dye (di-4-ANEPPDHQ) as a function of state in phospholipid vesicles and cell membranes. When the thermodynamic state of vesicles made from di-myristoyl-phosphatidylserine (DMPS) was changed by temperature or pH, the fluorescence intensity and spectrum of the embedded dye underwent characteristic changes. During the transition from the liquid-disordered to the liquid-ordered phase, the fluorescence intensity exhibited a maximum and the emission spectrum shifted to shorter wavelengths (by about 26 nm). Subsequently, the same dye was incorporated into the plasma membrane of an excitable cell (Chara Braunii). When an action potential was triggered the emission spectrum shifted to shorter wavelengths. This indicates that propagation of an action potential is associated with a significant change of state of the excitable cell membrane.

CPP 82.2 Fri 9:45 H 2013

Vesicle adhesion and fusion studied by small-angle x-ray scattering — •Karlo Komorowski[1], Annalena Salditt[1], Yihui Xu[1], Halenur Yavuz[2], Martha Brennich[3], Reinhard Jahn[2], and Tim Salditt[1] — [1]Institut für Röntgenphysik, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Department of Neurobiology, Max-Planck-Institute for Biophysical Chemistry, Göttingen, Germany — [3]European Molecular Biology Laboratory, Grenoble, France

Membrane fusion takes place in numerous physiological processes on the cellular and subcellular level as in the case of synaptic neurotransmission. The merger of two membranes generally involves a highly complex interplay on the molecular level among lipids, membrane fusion proteins, ions of the aqueous environment and water molecules. We aim at the structure of intermediate states of a vesicle and membrane fusion pathway. A main emphasis is laid on adhered vesicles. Recent observations indicate that such a docking state, showing two flattened membranes in close proximity, plays a role in vesicle fusion. For this purpose, we have studied adhesion and fusion of lipid vesicles induced by $CaCl_2/MgCl_2$, and show that a stable adhesion state can be induced under certain conditions. The bilayer structure and the inter-bilayer distance between adhered vesicles was analyzed by small-angle x-ray scattering (SAXS). From the obtained structural parameters we aim at an understanding of inter-membrane potentials in adhesion and in fusion. Finally, we have studied structural dynamics of lipid vesicle fusion using time-resolved SAXS techniques, and show that intermediate states can be distinguished over time.

Invited Talk CPP 82.3 Fri 10:00 H 2013

The role of dynamin twist in membrane fission — Martina Pannuzzo[1], Zachary A. McDargh[1,2], and •Markus Deserno[1] — [1]Department of Physics, Carnegie Mellon University — [2]Department of Chemical Engineering, Columbia University

The final step of many biological membrane fission events involves the GTPase dynamin, which assembles into a helical filament around the neck of a nascent vesicle and somehow severs this remaining connection. But despite about two decades of research, the actual physical processes that lead to fission are still a matter of debate. Dynamin's action occurs on the scale of a few tens of nanometers over just a few milliseconds, which is too small and fast for many experimental techniques, but too large and slow for atomistic simulations. Here we present coarse-grained simulations that are specifically designed to capture the interplay of geometry and elasticity. We argue that, within reasonable experimental limits, the two widely discussed conformational changes of shrinking the radius or increasing the pitch of a dynamin helix are insufficient to trigger fission. However, a third change, reminiscent of an effective twist of the filament, which accounts for the experimentally observed asymmetric unbinding of dynamin's PH-domains, turns out to efficiently drive the neck into the hemifission state. Following the retraction of the substrate, the remaining dynamin coat can unbind, and the tensile force in the connecting micellar string draws the almost severed membranes together one more time, until bilayer contact catalyzes the scission of the micelle.

CPP 82.4 Fri 10:30 H 2013

Appling forces to model cells using microfluidic systems — •Tom Robinson — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Biological cells in their natural environment experience a variety of external forces such as fluidic shear stress, osmotic pressures, and mechanical loads. While membrane proteins are a crucial part of the cellular response to external stimuli, in recent years so called *lipid rafts* have been thought to play an important role in the spatial organization of membrane proteins. Synthetic membranes such as giant unilamellar vesicles (GUVs) offer a reduced cell model, whereby individual components can be isolated and studied without interference from the complexity of the natural cell. However, applying specific forces to these delicate objects in a controllable manner is non-trivial. To this end, we report a microfluidic method to capture GUVs and apply a variety of forces. The first device contains micro-patterned electrodes which allows the application of electric fields and observations of the subsequent membrane fusion (Robinson et al. Lab on a chip 2014). The second device uses a valve-based system to apply specific fluidic shear forces to membranes (Sturzenegger et al. Soft Matter 2016). Our latest microfluidic design comprises an integrated micro-stamp which is able to mechanically compress GUVs to study the effects of deformation. We investigate the effects of these forces on the behaviour of lipid domains as a model for lipid rafts in cells.

CPP 82.5 Fri 10:45 H 2013

Design of a switchable DNA origami structure for shaping lipid membranes — •Alena Khmelinskaia[1], Megan Engel[2,3], Garima Mishra[3], Jonathan Doye[3], and Petra Schwille[1] — [1]Max Planck Institute of Biochemistry, Planegg, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, United Kingdom — [3]Department of Physical and Theoretical Chemistry, University of Oxford, Oxford, United Kingdom

Biological membranes are dynamic cellular barriers that suffer deformation and bending. In recent years, due to its exclusive nanoengineering properties, the DNA origami technology has been vastly used to build synthetic scaffolds that partially recapitulate curvature-inducing mechanisms. Nonetheless, the control over such shaping phenomena is yet scarce. Here, we design a DNA based nanostructure with an integrated conformational switch, with the goal to deform free-standing lipid membranes. Using site-directed single-strand displacement reactions as force elements, DNA nanostructures change their conformation into a bent state. Simulations of the DNA-based nanostructures using the oxDNA coarse-grained model confirm the experimentally observed bending. A complementary approach of nucleotide sequence variation and simulation is used to balance the implemented force elements and consequently optimize the conformational switch. We show that bent DNA-based structures are capable of inducing large scale deformations on free-standing lipid bilayers. Furthermore, our results may confirm theoretical predictions of membrane bending based on the free energy changes of the bound DNA structures.

CPP 82.6 Fri 11:00 H 2013

FCS analysis of protein mobility on lipid monolayers — •Jonas Mücksch[1,2], Alena Khmelinskaia[1,2], Franco Conci[1], Grzegorz Chwastek[1], and Petra Schwille[1] — [1]Max Planck Institute of Biochemistry, Am Klopferspitz 18, 82152 Martinsried — [2]authors contributed equally

In vitro membrane model systems are used to study complex biological phenomena under controlled unadulterated conditions. Lipid monolayers are particularly suited to study lipid packing in an unbiased manner. To explore the effect of lipid packing on protein mobility, we used miniaturized chambers instead of conventional Langmuir-Blodgett troughs. This assay requires only minute amounts of protein and is ideally suited to be combined with single molecule sensitive fluorescence correlation spectroscopy (FCS) to characterize diffusion dynamics. Our results confirm the influence of lipid packing on lipid mobility and validate the use of FCS as an alternative to conventional surface pressure measurements. Furthermore, we study the effect of lipid density on the diffusion of membrane binding biomolecules, ranging from small peptides to large DNA-based nanostructures. We exploit the sensitivity of FCS to characterize protein interactions with the lipid monolayer in a low concentration regime, which is inaccessible to conventional surface pressure measurements. Finally, we relate our measurements to the characteristic hydrodynamic length of the lipid monolayer. Our work provides a detailed strategy for the conduction of point FCS experiments on lipid monolayers, which is the first step towards extensive studies of protein-monolayer interactions.

CPP 82.7 Fri 11:15 H 2013

Structure and Conformation of Single and Interacting Bacterial Surfaces — •Ignacio Rodriguez Loureiro[1], Victoria Latza[1], Giovanna Fragneto[2], and Emanuel Schneck[1] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]Institut Laue-Langevin, Grenoble, France

The outer surfaces of Gram-negative bacteria are composed of lipopolysaccharide (LPS) molecules exposing oligo- and polysaccharides to the aqueous environment. This unique, structurally complex biological interface is of great scientific interest as it mediates the interaction of bacteria with antimicrobial agents as well as with neighboring bacteria in colonies and biofilms. Structural studies on LPS surfaces, however, have so far dealt almost exclusively with rough mutant LPS of reduced molecular complexity and limited biological relevance. Here, using neutron reflectometry we structurally characterize planar monolayers of wild-type LPS from Escherichia Coli O55:B5 featuring strain-specific O-side chains in the presence and absence of divalent cations and under controlled interaction conditions. For interacting LPS monolayers we establish pressure-distance curves and determine the distance-dependent saccharide conformation.

CPP 82.8 Fri 11:30 H 2013

Osmotic instabilities and organelle biogenesis — •Sami Al-Izzi[1,2], George Rowlands[2], Pierre Sens[1], and Matthew Turner[2] — [1]Institut Curie (UMR 168), Paris, France — [2]University of Warwick, Coventry, Uk

We study theoretically a membrane tube with unidirectional ion pumps driving an osmotic pressure difference. A pressure driven peristaltic instability is identified, quantitatively distinct from similar tension-driven Rayleigh type instabilities on membrane tubes. We discuss how this instability could be related to the function and biogenesis of membrane bound organelles, in particular the contractile vacuole complex found in protists. The unusually long natural wavelength of this instability is in close agreement with that observed in cells. We also consider extensions of this result to more complex/realistic systems.

CPP 82.9 Fri 11:45 H 2013

Cholesterol effects on lateral structure formation — •Fabian Keller, Davit Hakobyan, and Andreas Heuer — Institut für Physikalische Chemie, Münster, Deutschland

Cholesterol is essential for, e.g. , the domain formation of lipid membrane mixtures and is thus at the heart of many basic properties of lipid membranes.

In recent studies we could show that cholesterol is able to intercalate between DPPC molecules without changing the mean distance of their head groups and, surprisingly, not changing the number of DPPC or DLiPC neighbors. Additionally the presence of cholesterol was found to decrease the lipid-lipid interactions of nearby lipids, indicating the complex interaction mechanisms in cholesterol containing bilayers. Our findings support the observations of cholesterol's condensing capabilities and DPPC-cholesterol interaction to be the driving force for domain formation.

To further understand the underlying mechanisms of cholesterols unique properties it is an essential step to include cholesterol to a formerly introduced Monte Carlo lattice model mapping MD data of DPPC and DUPC bilayers to a lattice [1]. Using this model one will be able to study cholesterol structure formation for decisively greater length and time scales, thereby completely resorting to input from short-time MD data.

[1] D. Hakobyan, A. Heuer, J. Chem. Phys. 146, 064305 (2017)

CPP 83: 2D Materials (Symposium and Joint Session with HL and O): Session III (joint session DS/CPP/HL)

Time: Friday 9:30–12:30 Location: H 2032

Invited Talk CPP 83.1 Fri 9:30 H 2032

Tunable Electronic Structures, Magnetism, and Axis-Dependent Conduction Polarity in Ge and Sn-based 2D Materials — •Joshua Goldberger — The Ohio State University, Columbus, OH USA

Here, we will discuss recent developments in the synthesis, properties, and applications of two classes of Ge- and Sn-based 2D materials; the ligand-functionalized Ge/Sn graphane analogues, and the exfoliatable van der Waals Zintl phases. First, the Ge/Sn graphane analogues have generated much excitement as their electronic structures are predicted to range from trivial insulators, to semiconductors with tunable gaps, to semimetallic, to topological insulators, depending on the substrate, chemical functionalization and strain. Through the synthesis and characterization of a large family of ligand-functionalized germananes, we will show how the electronic structure can be manipulated via surface chemistry. Second, we will highlight a new family of chemically and thermally robust exfoliatable 2D materials having a stoichiometry of ASn2Pn2, where A is a cation, and Pn is a pnictogen. This class of materials can be designed to exhibit a broad range of phenomena including the topological insulating compound, SrSn2As2, as well as the magnetic compound, EuSn2As2. Also, we will show that NaSn2As2 simultaneously exhibits opposite sign conduction polarities along its in-plane and cross-plane axes. Using a variety of advanced transport measurements we establish the band structure origins of this behavior. Together, these materials show how the inherent anisotropy in 2D materials can be rationally tailored to give rise to new phenomena.

CPP 83.2 Fri 10:00 H 2032

Chemical and optical properties of transition metal dichalcogenide monolayers at the nanometer and subnanometer scale — •Luiz Tizei[1], Alberto Zobelli[1], Ching-Hwa Ho[2], Kazu Suenaga[3], Alexandre Gloter[1], Mathieu Kociak[1], and Odile Stéphan[1] — [1]Laboratoire de Physique des Solides, University of Paris-Sud, CNRS, Orsay, France — [2]National Taiwan University of Science and Technology, Taipei, Taiwan — [3]AIST, Tsukuba, Ibaraki, Japan

Defects and interface play an important role in material properties. Therefore, their characterization at the nanometer scale is crucial. Here, core-loss EELS and high angle annular dark field imaging have been used to identify single Cr atoms in WSe_2 monolayers. These atoms are always located at the metal site (W) with a 3+ formal valence, as deduced from EELS fine structure comparison with known references and X-ray photoelectron spectroscopy (XPS). Furthermore, Cr atoms are observed systematically close to single our double Se vacancies, indicating a possible electron doping of the system. Moreover, semiconducting 2H phase TMD monolayers present spin-split valence and conduction bands due to spin-orbit coupling. These two near band edge states are separated by from a few tens to a few hundred meV and can be measured by EELS with high spatial resolution. As an example, we will show measurements of the near band edge losses as a function of position across an interface between two TMDs. Results will be compared to calculated loss functions, tacking into account the materials' dielectric function.

CPP 83.3 Fri 10:15 H 2032

Excitonic Phonon Sidebands in Monolayer Transition Metal Dichalcogenides — •Dominik Christiansen[1], Malte Selig[1], Gunnar Berghäuser[2], Robert Schmidt[3], Iris Niehues[3], Robert Schneider[3], Ashish Arora[3], Steffen Michaelis de Vasconcellos[3], Rudolf Bratschitsch[3], Ermin Malic[2], and Andreas Knorr[1] — [1]Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, Gothenburg, Sweden — [3]Physikalisches Institut und Zentrum für Nanotechnologie, Universität Münster, 48149 Münster, Germany

Monolayers of transition metal dichalcogenides (TMDs) show an extraordinarily strong Coulomb interaction, leading to the formation of tightly bound excitons. Because of a complex quasi-particle band structure, TMDs possess a variety of bright sates (addressable by light) and dark states (addressable by phonons). Here, we present a joint experiment-theory study on the influence of exciton-radiative and exciton-phonon interaction on the absorption line shape of different monolayer TMD materials. Solving the TMD Bloch equations in the quantum kinetic limit, we predict the appearance of spectrally asymmetric phonon-induced sidebands that are accompanied by a pronounced polaron-red shift. We analyze the influence of the interplay of phonon emission/absorption processes and dark intra- and intervalley excitonic states on the asymmetry of the absorption line shape.

D. Christiansen, et. al, Phys. Rev. Lett. 119, 187402 (2017)

CPP 83.4 Fri 10:30 H 2032

Lifetime of Valley Excitons in Monolayer Transition Metal Dichalcogenides — •Malte Selig[1], Samuel Brem[2], Florian Katsch[1], Gunnar Berghäuser[2], Ermin Malic[2], and Andreas Knorr[1] — [1]Nichtlineare Optik und Quantenelektronik von Halbleitern, Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, Gothenburg, Sweden

In monolayers of transition metal dichalcogenides, weak screening leads to the formation tightly bound excitons which dominate the optical properties of these ultrathin materials. A pronounced circular dichroism leads to a spin and valley selective excitation of excitons at the corners of the hexagonal Brillouin zone. A microscopic understanding of the lifetime of such optically injected spins is of crucial interest for future technological applications. Here, based on a Heisenberg of motion formalism for excitons, we perform microscopic momentum and spin resolved computations to investigate the impact of exciton phonon coupling and intervalley exchange coupling on the valley lifetime of excitons. In our analysis, we also include recently discussed indirect dark excitons [1,2]. In the absence of low lying dark states we find valley lifetimes below 1 ps, which increases by orders of magnitude if the material is indirect.

[1] M. Selig et al., Nat. Commun. 7, 13279 (2016)

[2] M. Selig et al., arXiv:1703.03317 (2017)

CPP 83.5 Fri 10:45 H 2032

Interface sensitive structure determination of silicon nanoribbons on Gold surfaces — •Peter Roese[1,2], Philipp Espeter[1,2], Karim Shamout[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik 1, Technische Universität Dortmund, Germany — [2]DELTA, Technische Universität Dortmund, Germany

In the last years there has been much progress in the growth and analysis of 2D-materials beyond graphene on metallic surfaces. Especially, silicon based two-dimensional silicene and one-dimensional silicon nano-ribbons came into scientific focus due to their promising electronic properties. Beside the exact knowledge of the fascinating electronic and chemical properties of such systems, the structural information is of great interest for precise DFT calculations. In this context the interaction between the silicon nano-ribbons and the substrate plays an important role. Techniques like STM or LEED provide information about the electronic structure of such systems but neither chemical information about the atomic bonds nor information about the interface. Photoelectron spectroscopy and diffraction easily provide information about atomic bonds and the interface between silicon nano-ribbons and the substrate, recently shown by Espeter et al [8]. The structure of silicon nano-ribbons on Ag(110) has recently been resolved whereas their exact structure on Au(110) and the effect of the interface needs to be analyzed in detail. Based on previous works, we present first photoelectron diffraction results of silicon nano-ribbons on Au(110).

15 min. break.

CPP 83.6 Fri 11:15 H 2032

Disclosing the nature of excitons in van der Waals materials: The role of layer stacking in hexagonal boron nitride — •Wahib Aggoune[1,2], Caterina Cocchi[2,3], Dmitrii Nabok[2,3], Karim Rezouali[1], Mohamed Akli Belkhir[1], and Claudia Draxl[2,3] — [1]Laboratoire de Physique Théorique, Faculté des Sciences Exactes, Université de Bejaia, 06000 Bejaia, Algeria — [2]Institut fur Physik and IRIS Adlershof, Humboldt-Universitat zu Berlin, Berlin, Germany — [3]European Theoretical Spectroscopic Facility (ETSF)

With the example of bulk hexagonal boron-nitride, a prototypical van der Waals (vdW) crystal, we demonstrate that the electronic and optical properties of these materials can be tuned by layer patterning. By modifying the stacking, energy, intensity, and character of the electron-hole (e-h) pairs can be selectively modulated. Depending on the specific layer arrangement, lowest-energy excitons are localized within a single layer or delocalized in the three-dimensional space. Only in specific stackings charge-transfer e-h pairs appear above the absorption onset, triggered by the spatial distribution of the electronic states involved. Our results, obtained within a first-principles many-body framework, provide all the ingredients to identify, predict, and tailor the character of the e-h pairs in vdW materials.

CPP 83.7 Fri 11:30 H 2032

Evidence for low-dimensional charge transport in carbon nitride polymers — •Christoph Merschjann — Helmholtz-Zentrum-Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

Carbon nitride (CN) polymers have gained much interest in recent years due to their potential application as both dark- and photocatalysts for various renewable-energy tasks, including water-splitting and CO_2 reduction, and others. Given their layered, van-der-Waals bound structure, these materials resemble graphite, and are hence often called "graphitic carbon nitrides" (g-C_3N_4). The main technical advantage of CNs is the abundance of their constituents (C, N, and H) and the absence of precious metals. However, compared to metal-based catalysts, the activity of CN materials is still rather low, a fact that has been largely attributed to their low conductivity. Recently, we found evidence that this low conductivity is due to polaronic hopping motions of photoexcited electrons and holes, which predominantly move vertical to the graphitic planes of the material. Backed-up by very recent transient-spectroscopy studies, we will discuss the validity of such a low-dimensional transport scenario, and its consequences for applications in catalysis as well as in organic electronics in general.

CPP 83.8 Fri 11:45 H 2032

Deterministic Positioning of Single-Photon Emitters in Monolayer WSe$_2$ on the Nanoscale — •Johannes Kern[1], Iris Niehues[1], Philipp Tonndorf[1], Robert Schmidt[1], Daniel Wigger[2], Robert Schneider[1], Torsten Stiehm[1], Steffen Michaelis de Vasconcellos[1], Doris E. Reiter[2], Tilman Kuhn[2], and Rudolf Bratschitsch[1] — [1]Institute of Physics and Center for Nanotechnology, University of Münster, Germany — [2]Institute of Solid State Theory, University of Münster, Germany

Single-photon emitters are an important building block for photonic quantum technology. Here, we deterministically position single-photon emitters in monolayer WSe$_2$ on the nanoscale [1]. The atomically thin semiconductor is placed on top of a gapped single-crystalline gold rod which results in a folding of the monolayer around the metal nanostructure. At the gap position, local strain is induced in the atomically thin semiconductor. Excitons localize there and radiatively decay via single-photon emission.

[1] J. Kern et al., "Nanoscale positioning of single-photon emitters in atomically thin WSe2", Adv. Mater. 28, 7101-7105, (2016).

CPP 83.9 Fri 12:00 H 2032

Pulsed Laser Deposition of Monolayer WSe$_2$ — •Avaise Mohammed[1], Hiroyuki Nakamura[1], Peter Wochner[1], Shyjumon Ibrahimkutty[1], Armin Schulz[1], Kathrin Müller[1], Krystian Nowakowski[2], Keita Matsuda[3], Johannes Geurs[1], Yijin Zhang[1], Mona Stadler[4], Kenji Watanabe[5], Takashi Taniguchi[5], Benjamin Stuhlhofer[1], Georg Cristiani[1], Gennady Logvenov[1], Michael Jetter[4], Peter Michler[4], Jurgen Smet[1], Ulrich Starke[1], and Hidenori Takagi[1,6] — [1]MPI-FKF — [2]University of Twente — [3]Nagoya University — [4]IHFG, University of Stuttgart — [5]NIMS — [6]IFMQ, University of Stuttgart

Ultrathin WSe$_2$ films were deposited using a custom built hybrid-Pulsed Laser Deposition (PLD) system on different substrates. Raman spectroscopy and atomic force microscopy were used to identify the monolayer (ML) WSe$_2$. Synchrotron based grazing incidence X-ray diffraction revealed WSe$_2$ films to have a compressive strain on Al$_2$O$_3$ r-cut substrates. Angle resolved photoelectron spectroscopy confirmed the valance band structure of ML WSe$_2$ on epitaxial graphene with a clear spin splitting of 480 meV. Photoluminescence signal was identified from ML WSe$_2$ deposited on hexagonal BN. The results give evidence for PLD to be an excellent approach for the growth of monolayer transition metal chalcogenides.

CPP 83.10 Fri 12:15 H 2032

Gate-dependent spin dynamics of dark trion states in monolayer WSe$_2$ — •Manfred Ersfeld, Frank Volmer, Maximilian Heithoff, Christopher Franzen, Christoph Stampfer, and Bernd Beschoten — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany

We explore the spin dynamics in WSe$_2$ monolayers by time-resolved Kerr rotation measurements. The longest spin lifetimes of up to 150 ns are observed at 5 K when resonantly pumping into charged exciton states (trions). We explain these long spin lifetimes by the formation of dark trion states which exhibit equal recombination lifetimes independently measured by time-resolved reflectivity [1]. We show that the spin lifetimes of the dark trion states strongly depend on the chemical potential which we tune by applying a gate voltage to the WSe$_2$ flake through a SiO$_2$/Si^{++} substrate. The formation of the dark trion states require intervalley scattering driven by short range scattering centres. Additional photoluminescence measurements indicate that this short range scattering is caused by localized states and gets strongly diminished with increasing temperature which may also be relevant for the overall strong decrease of both the spin amplitude and the spin lifetime of the dark trion states with increasing temperature.

[1] F. Volmer et al., Phys. Rev. B 95, 235408 (2017)

CPP 84: Glasses and Glas transition (joint session DY/CPP)

Time: Friday 10:00–12:45 Location: BH-N 334

CPP 84.1 Fri 10:00 BH-N 334

Can the glass transition occur in non-equilibrium? — •Michael Schmiedeberg — Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Recently, there have been great advances in the simulation of equilibrated hard sphere systems up to high densities that can even exceed the athermal jamming packing fraction (see, e.g., [1]). As a consequence, several researchers claim that all previous simulations were obsolete and that it even was not allowed to do further studies of non-equilibrium systems.

In my contribution I want to motivate that by limiting the research to systems in equilibrium one misses important and interesting phenomena that exist in non-equilibrium systems, e.g., ageing, avoidance of crystallization, history-dependence, as well as many other properties of the dynamical glass transition and of glasses. I argue that dynamical glasses obtained by rapid quenches can be significantly different from ideal, structural glasses that might occur in equilibrated systems.

[1] A. Ninarello, L. Berthier, and D. Coslovich, Phys. Rev. X 7, 021039 (2017).

CPP 84.2 Fri 10:15 BH-N 334

Nonlinear response theory: simple stochastic models — •Gregor Diezemann — Institut für Physikalische Chemie, Universität Mainz

The effect of large electric fields on the relaxation of supercooled liquids and also other systems like ionic liquids and crystals has been studied intensively during the last decade. Due to the formal lack of an analogue to the well known fluctuation dissipation theorem valid for linear response, one essentially relies on model calculations in the nonlinear case. There are a number of different models that have been used to compute the nonlinear response of glassforming systems, such as the so-called box model, the model of isotropic dipole reorientations or the dipole flips in an asymmetric double well potential (ADWP). I will discuss the results of model calculations of the nonlinear response for simple stochastic models for the dynamics. In particular, I will consider the ADWP model which is known to exhibit a peak in the modulus of the third-order response in a narrow temperature range around some characteristic temperature. Interestingly, in fifth order one observes peaks in the modulus around two characteristic temperatures. These peaks are related to the vanishing of the nonlinear static susceptibility in the respective order. The results will be discussed in the light of recent experimental observations.

CPP 84.3 Fri 10:30 BH-N 334

Lokaler Debye-Prozess? Einblicke in 1-Propanol mit Hilfe der Triplett-Solvatationsdynamik — •Daniel Koestel[1], Peter Weigl[2], Thomas Blochowicz[2] und Thomas Walther[1] — [1]TU Darmstadt, Institut für Angewandte Physik — [2]TU Darmstadt, Institut für Festkörperphysik

Mit Hilfe der Triplett-Solvatationsdynamik (TSD) ist es möglich das Relaxationsverhalten unterkühlter Flüssigkeiten und auch in geometrisch eingeschränkten Systemen lokal zu untersuchen [1]. Dabei wird ein Farbstoff in geringer Konzentration in der Probe gelöst und mittels eines UV-Laserpulses in einen langlebigen Triplett-Zustand angeregt. Durch die Relaxation der den Farbstoff umgebenden Moleküle kommt es zu einer Rotverschiebung des vom Farbstoff emittierten Spektrums. Diese zeitabhängige Stokes-Verschiebung kann zur Bestimmung des lokalen Relaxationsverhaltens der Solvationshülle genutzt werden [1]. Wasserstoffbrückenbildende Flüssigkeiten sind von besonderem Interesse, da diese auch in biologischen Systemen eine zentrale Rolle einnehmen. Besonders Monohydroxy Alkohole weisen dabei in der dielektrischen Spektroskopie den prominenten Debye-Prozess auf [2], dessen mikroskopischer Ursprung nach wie vor Gegenstand kontroverser Diskussion ist und meist der Relaxation einer transienten, supermolekularen Kettenstruktur zugeschrieben wird, die sich aufgrund von Wasserstoffbrücken ausbildet [3]. Dabei gehen wir der Frage nach, ob und wie diese Kettendynamik von einer lokalen Sonde detektiert wird.

[1] R. Richert. J. Chem. Phys. 113 (2000) [2] J. Gabriel et al. J. Phys. Chem. B 121 (2014) [3] R. Böhmer et al. Phys. Rep. 545 (2014)

CPP 84.4 Fri 10:45 BH-N 334

Analytical solution of the spin model on the Bethe lattice — •Koray Önder[1,2], Till Kranz[1,2], and Matthias Sperl[1,2] — [1]Institut für Theoretische Physik, Uni Köln — [2]Institut für Materialphysik im Weltraum, DLR Köln

The cooperative facilitation scenario (CFS) on the Bethe lattice shows similarities in the correlation functions with the mode coupling theory (MCT). The first studies by fitting some critical exponents on the CFS are in good agreement with the MCT predictions [1].

The fact that the CFS on the Bethe lattice yields a bifurcation scenario can be used to describe the asymptotic dynamics of the system. As a result we obtain analyticaly exact predictions for the critical exponents and the master function.

[1] M. Sellitto, Phys. Rev. Lett. **115**, 225701 (2015)

CPP 84.5 Fri 11:00 BH-N 334

Structure and dynamics of water-like models — •Robin Horstmann and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt, Germany

Among glass-forming liquids tetrahedral network formers like water have a special position. Their vast amount of anomalies make the transfer of models like density scaling difficult. We thus use molecular dynamics simulations to examine a family of water-like molecules produced by systematically varying the partial charges of the SPC/E and TIP4P2005 water models [1]. The geometry of the molecules remains unchanged but the inter-molecular interactions of the models vary strongly. We show that the resulting dynamics spread over a wide temperature range with the glass transition temperature T_g and the high temperature activation energy E_∞ both changing by a factor of five. Models of the glass transition are tested using observables from these studies on water-like models in the bulk and from concomitant work on these systems in confinement which allows us to determine structural and dynamical length scales. Common behavior of the models can be found using a recently proposed empirical function that splits the activation free energy into a constant value E_∞ and an exponentially growing contribution $E_c(T)$ [2]. A common ratio of E_∞/T_g is found. Modification of the partial charges also changes the phase diagram preparing the ground for studies of water's two supercooled phases.

[1] Horstmann, R., and M. Vogel. J Chem Phys **147**, 034505 (2017)
[2] Schmidtke, B. et al., Phys. Rev. E **86**, 041507 (2012)

CPP 84.6 Fri 11:15 BH-N 334

Secondary Relaxation Dynamics Observed by Photon-Correlation-Spectroscopy — •Till Böhmer, Jan Gabriel, Andreas Helbling, Florian Pabst, and Thomas Blochowicz — TU Darmstadt, Institut für Festkörperphysik, Germany

Secondary relaxation processes in simple molecular glass formers have been a long-standing topic in research of supercooled liquids and amorphous solids. In particular understanding the mechanism behind Johari-Goldstein-β-relaxation is considered to be important, because it originates from the dynamic of the entire molecule and is expected to be a universal feature of the glass-transition.

To obtain a new perspective, photon-correlation-spectroscopy (PCS) was utilized to examine reorientational dynamics in various monohydroxy alcohols. After improvements regarding the experimental setup secondary relaxation processes were successfully resolved in PCS. By comparing the results of light scattering experiments with those of broadband dielectric spectroscopy, focusing on the differences in amplitude and shape of the respective processes, insight on the mechanism behind the JG-β-relaxation can be gained.

15 min. break

CPP 84.7 Fri 11:45 BH-N 334

Emergent Many-body Interactions and Inapplicability of Hard Sphere Jamming Theory — •Yoav G. Pollack[1], Murari Singh[1], Giorgio Parisi[2], Corrado Rainone[1], and Itamar Procaccia[1] — [1]Weizmann Institute of Science, Israel — [2]Sapienza Universit di Roma, Italy

The mechanism of jamming in soft matter was recently argued to be dimensionally independent by studying the scaling exponents predicted within an infinite-Dimensional mean-field hard-sphere theory. The predicted critical exponents were found to match surprisingly well the numerical measurements in finite-D including 2D and 3D. Such a match seemingly suggests that the infinite-D theory is applicable to realistic systems. Our current work addresses the puzzle of this lack of strong D dependence usually observed in critical phenomena.

We study the jamming transition using *effective* inter-particle forces. In thermal materials where nevertheless the mean positions are well defined on a given time-scale, these effective forces are what keeps the particles "in place". We observe emergent effective many-body forces, and quantify the non-binary contributions Vs. proximity to jamming. For hard spheres the effective forces are binary *precisely* at jamming, similarly to the infinite-D limit and propose that this explains the match of theory and measurements. We further conclude that the predictions of infinite-D hard spheres should not be inapplicable to more realistic particles which are never absolutely hard[1].

[1]G. Parisi, Y.G. Pollack, I. Procaccia, C. Rainone and M. Singh, Submitted for publication, arXiv:1709.01607.

CPP 84.8 Fri 12:00 BH-N 334

Controlled crystallization of luminescent lithium borate glasses — •A. Charlotte Rimbach[1], Juliane Schuppich[1], Bernd Ahrens[1,2], Franziska Steudel[2], and Stefan Schweizer[1,2] — [1]South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest — [2]Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Microstructure of Materials and Systems IMWS, Lübecker Ring 2, 59494 Soest

Lanthanide-doped borate glasses are promising candidates as frequency-converter for LED applications. The borate glass system provides high transparency in the visible spectral range, good lanthanide ion solubility and high mechanical stability. The lanthanide ions terbium (Tb^{3+}) and europium (Eu^{3+}) show a bright luminescence therein with quantum efficiency values of approx. 60 % (486 nm excitation) and 90 % (396 nm excitation), respectively. However, since the absorption coefficient of the lanthanide ions is low, only a small amount of the excitation light is absorbed resulting in a poor conversion efficiency. To increase the optical absorption by prolonging the optical pathway through multiple scattering within the glass, the as-made luminescent borate glasses are processed to glass ceramics. The focus of this work is on the analysis of the crystallization process by means of differential scanning calorimetry (DSC), in situ x-ray diffraction (XRD) as well as optical spectroscopy and quantum efficiency (QE) measurements.

CPP 84.9 Fri 12:15 BH-N 334

Glassy dynamics as reflected in its inter- and intra-molecular interactions — •Friedrich Kremer, Wilhelm Kossack, and Markus Anton — Institute of Experimental Physics I, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

The inter- and intra-molecular interactions of low molecular weight and polymeric glass-forming model systems are studied by Broadband Dielectric (BDS) - and Fourier-Transform Infrared (FTIR) - Spectroscopy. Analyzing the temperature dependencies of specific IR absorption bands, reflecting the intramolecular potentials of dedicated molecular moieties, enables one to unravel on an intramolecular scale the process of glass formation and to compare it with the dielectrically determined primarily intermolecular dynamics. Molecular systems to be studied are typical glassformers as glycerol, propyleneglycol, polypropyleneglycol, propylenecarbonate and polypropylencarbonate. By that a wealth of novel information is obtained proving that the different molecular moieties of a glass former show often strongly different characteristic, temperature dependencies. This demonstrates the fundamental importance of intra-molecular dynamics giving refined insights into the underlying interactions beyond coarse-grained models treating the glassformer as rigid body.

CPP 84.10 Fri 12:30 BH-N 334

Site energy distributions in ion conducting glasses — •Martin Schäfer and Karl-Michael Weitzel — Philipps-Universität Marburg, Marburg, Germany

In a crystalline sample of an ion-conducting material all ions exhibit the same surrounding and thus the same site energy. In an ion-conducting glass ions exhibit different local surroundings. Thus, a distribution of site energies will apply. So far all information on such site energy distributions appears to either come from theory or indirect experiments. This site energy distribution is evidently crucial for all transport processes involving the transport of considerable fractions of mobile ions, e.g. in battery materials. Consequently, direct information on this energy distribution best comes from an experiment, where all ions of a certain kind are almost completely depleted, e.g. by a foreign ion. By reanalysis of previously published concentration depletion profiles within the foreign ion bombardment induced ion transport [1] we are now able to derive the complete site energy distribution of sodium ions in a calcium-sodium-phosphate glass. The occupied part of the site energy distribution spans a width of about 0.28 eV FWHM [2].

[1]*L. Rossrucker, P.V. Menezes, J. Zakel, M. Schäfer, B. Roling and K.-M. Weitzel, Zeitschrift für Physikalische Chemie, 226, 341-353, (2012).

[2]*M. Schäfer, K.-M. Weitzel, to be submitted

CPP 85: Molecular films: Photovoltaics, electronics and morphology (joint session O/CPP)

Time: Friday 10:30–11:30 Location: MA 144

CPP 85.1 Fri 10:30 MA 144

Excitonic states in films of 1,3-diphenylisobenzofuran — •Janek Rieger, Daniel Niesner, and Thomas Fauster — Lehrstuhl für Festkörperphysik, University of Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

Films of 1,3-diphenylisobenzofuran (DPIBF) show singlet fission (SF), a mechanism for multi-exciton generation that might be used to enhance the efficiency of organic photovoltaics [1]. The yield of singlet fission depends strongly on the structural polymorph of the film [2]. We use ultraviolet photoelectron spectroscopy, monochromatic two-photon photoelectron spectroscopy, photoluminescence (PL) spectroscopy and time-resolved PL to investigate the occupied molecular orbitals and excitonic behavior in different polymorphs of DPIBF on Cu(111). Preparations under ultra-high vacuum conditions provided well-defined samples, on which in-situ measurements were carried out. In disordered films an excimer trapping state with a lifetime of 50 ns was found with an energy ~ 0.5 eV below the first excited singlet state S_1. For ordered films additional three vibrational progressions were found, which can be attributed to the S_1 excitons of two different polymorphs with energies of 2.62 eV and 2.66 eV and an emissive triplet pair species with an energy of 2.72 eV. The latter decays with two time constants in the subnanosecond regime. A relative PL yield < 0.12 was determined for the ordered films, which points towards a highly SF active film.

[1] M. C. Hanna, and A. J. Nozik, J. Appl. Phys. **100**, 074510 (2006).

[2] J. L. Ryerson et al., J. Phys. Chem. C **118**, 12121-12132 (2014).

CPP 85.2 Fri 10:45 MA 144

Polarized-Light Induced Contact Potential Differences in Small-Molecule Organic Aggregates and Thin Films — •Frank Balzer[1], Matthias Schulz[2], Oliya S. Abdullaeva[3], Arne Lützen[2], and Manuela Schiek[3] — [1]University of Southern Denmark, MCI, Sønderborg, Denmark — [2]University of Bonn, Germany — [3]University of Oldenburg, Germany

Crystalline organic thin films often exhibit linear dichroism and birefringence. Illumination with polarized light might therefore lead to polarization dependent changes of the electric surface potential. Here, we present results for birefringent and dichroic nanofibers from functionalized *para*-quaterphenylene molecules [1], and for thin films and thin film blends from an dihydroxy anilino squaraine (SQIB) [2]. Considerable differences in the light-induced changes of the surface potential are observed, probed by Kelvin probe force microscopy (KPFM). These changes are associated with the local molecule orientation within the samples.

[1] J. Chem. Phys. 146 (2017) 134704. [2] Cryst. Growth Des. (2017), doi: 10.1021/acs.cgd.7b01131.

CPP 85.3 Fri 11:00 MA 144

Work function variation due to electron induced conversion of self-assembled monolayers into carbon nano-membranes — Paul Penner[1], •Sascha Koch[1], Marcin Kiesiel[2], Thilo Glatzel[2], Emanuel Marchewski[1], Xianghui Zhang[1], Ernst Meyer[2], and Armin Gölzhäuser[1] — [1]Faculty of Physics, University of Bielefeld, 33615 Bielefeld, Germany — [2]Department of Physics, University of Basel, 4056 Basel, Switzerland

For the realization and improvement of molecular electronic devices as for instance nano capacitors, the determination and specific tuning of electrical properties of the build-in materials plays an important role [1]. Our main research is focused on Carbon nano-membranes (CNMs), made by e.g. electron irradiation induced cross-linking of self-assembled monolayers (SAMs) of aromatic, organic molecules. Using different precursor molecules for the SAM preparation allows us to tune various properties of the resulting CNM [2]. Here, we present a material study about the change in the work function of pristine SAMs and CNMs on a Au(111) substrate by means of Kelvin Probe Force Microscopy (KPFM) for different precursor molecules. For different samples, the morphology as well as the work function of partially cross-linked and pristine SAM areas were compared, showing only differences in the contact potential (CPD). This effect can be attributed to the dipole moment modification of the molecular layer as well as the molecule-substrate interface but also to influences of different headgroup functionalizations. [1] X. Zhang et al., J.Appl.Phys. 2017, 122, 055103. [2] A. Turchanin et al., Adv. Mater. 2016, 28, 6075-6103.

CPP 85.4 Fri 11:15 MA 144

Local near-field spectroscopy of squaraine J-aggregates — •Jinxin Zhan, Jens Brauer, Manuela Schiek, Petra Gross, and Christoph Lienau — Carl von Ossietzky Universität, Oldenburg, Germany

Investigating the relationship between structure and function of organic molecular systems is of great interest for understanding their optical and electronic properties, inter- and intra-molecular coupling, and further applications such as solar cells, transistors, and photovoltaic devices. Optical microscopy on a nanometer length scale is one promising approach to obtain such insights. Here we employ scattering-type near-field scanning optical microscopy (NSOM) to probe the local spectrum of squaraine J-aggregates (R-ProSQ-C16). We model two resonances in the far-field spectrum of the molecules as transitions from the ground state to two excited states which originate from the energy level splitting caused by the coupling between two adjacent monomers. The splitting strength and hence the transition energy is determined by the tilt angle between the two coupled monomer dipoles. Near-field spectral measurements resolve local scattering spectra in 10-nm-radius domains. They reveal that the resonance energies measured in the individual domains vary from each other. These near-field spectral measurements, in combination with our theoretical modelling, reveal local variations in the tilt angle between the two monomer dipoles.

CPP 86: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VIII (joint session O/TT/MM/DS/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Friday 10:30–12:45 Location: HL 001

CPP 86.1 Fri 10:30 HL 001

Ab initio photoluminescence in 2D materials — •Pedro Melo[1,4], Andrea Marini[2,4], Matthieu Verstraete[1,4], and Zeila Zanolli[3,4] — [1]NanoMat / CESAM, ULiege Belgium — [2]ISM CNR, Italy — [3]RWTH Aachen Germany — [4]ETSF

The theoretical study of photoluminescence (PL) has been hindered in the past due to lack of predictive ab initio numerical techniques [1,2,4]. We present a complete theoretical framework for the computation of PL where electrons, nuclei, and photons are quantised. The intrinsic non-equilibrium nature of the process is fully taken into account [3]. Starting from the Keldysh contour, we arrive at a set of equations for the Green's functions of electrons, phonons, and photons where the different kinds of interactions are treated on the same footing. These equations are then simplified by using the generalised Baym-Kadanoff ansatz and the completed collision approximation [3]. This reduces the problem to a set of decoupled equations for the density matrix that describe all kinds of static and dynamical correlations. We show how the micro-macro connection relates the observable spectrum with the time-dependent microscopic dynamics, via the Bethe-Salpeter equation. Finally, we present the results of our numerical studies on 2D materials, such as WS2, where we relate the evolution of the carrier populations in the Brillouin zone with the changes in the PL spectrum of the material, for a range of experimental setups. [1] M. F. Pereira and K. Henneberger, PRB 58, 2064 (1998). [2] K. Hannewald, et al, PRB 67, 233202 (2003). [3] P. M. M. C. de Melo and A. Marini, PRB 93, 155102 (2016). [4] S. W. Koch, et al, Nat Mat 5, 523 (2006).

CPP 86.2 Fri 10:45 HL 001

Strain on molybdenum disulfide sheets with defects from first principles — •Mohammad Bahmani[1], Mahdi Faghihnasiri[2], and Thomas Frauenheim[1] — [1]BCCMS, Physics Department, Bremen University, Bremen, Germany — [2]Physics Department, Shahrood University of Technology, Shahrood, Iran

Single layer of transition metal dichalcogenides(TMDCs) are under intense investigations since the discovery of unique characteristics of 2D and Vann der Waals layered materials. They are predicted to be the most promising structure for various future nanoscale devices. They have also novel applications in spintronic and optoelectronic. As a result of thermal equilibrium and the kinetics of processing, all real materials contain structural defects which show significant effects on their electrical, optical, vibrational, magnetic, and chemical properties. Besides, mechanical strain has very much influence on the electronic properties of 2D materials, particularly TMDCs. For example, 0.5% biaxial strain force direct band gap in molybdenum disulfide(MoS2) to become indirect since it breaks the crystalline symmetry. Therefore, I study different types of point defects such as single and double sulfur(S), single molybdenum(Mo) vacancies, and removing a Mo with its three upper S neighbors. I also substitute a Mo vacancy with one and two S atoms. Furthermore, as the second aim of this study, I showed the modification of defect states under uniaxial and biaxial compression and tensile strain. For the case of one S vacancy, this moves shallow states into the valance band and importantly breaks the degeneracy of degenerate states.

CPP 86.3 Fri 11:00 HL 001

Competion of magnetic interactions and in-field behavior of cycloidal Uranium compound UPtGe. — •Leonid Sandratskii — Max Planck Institute of Microstructure Physics, Halle, Germany

Stimulated by recent high-field experiment [1] performed on unique actinide system with cycloidal magnetic structure, UPtGe, I performed a series of calculations aiming to understand the nature of the sequence of magnetic phase transitions caused by the applied magnetic field. The physics of the system is determined by the fine balance of the exchange interaction, magnetic anisotropy, and Dzyaloshinskii-Moriya interaction. This balance of interactions governs, in particular, the in-field behavior of the system. The physical consequences of the variation of the localization of the U 5f electrons is investigated.

[1] A. Miyake, A. Nakamura, Y. Shimura, Y. Honma, D. Li, F. Honda, M. Tokunaga, D. Aoki, doi.org/10.11316/jpsgaiyo.71.1.0_2062.

CPP 86.4 Fri 11:15 HL 001

Electron correlation effects in the electronic structure of 4f-atoms adsorbed on metal and Graphene substrates — •Alexander B. Shick[1], Dmitry S. Shapiro[2], and Alexander I. Lichtenstein[3] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [2]nstitute of Radio Engineering and Electronics, Russian Academy of Sciences, Moscow — [3]Institute of Theoretical Physics, University of Hamburg, Germany

Surface supported single magnetic atoms, the so-called "single-atom magnets", open new opportunities in a quest for the ultimate size limit of magnetic information storage. Initially, the research mainly focused on 3d-atoms on surfaces. Recently, the attention was turned to the 4f-atoms, culminating in the experimental discovery of magnetically stable Ho atom on MgO(001) substrate [1], and Dy atom on graphene/Ir(111)[2]. We address the electronic and magnetic character of 4f-atoms on metal and Graphene substrate making use of a combination of the DFT with the exact diagonalization of Anderson impurity model (DFT+ED) [3]. The spin and orbital magnetic moments of Dy@Ir(111) and Dy/Graphene/Ir(111) are evaluated and compared with experimental XMCD data. The magnetic anisotropy energy is estimated, and the magnetic stability is discussed. The role of 5d-4f interorbital exchange polarization in modification of the 4f-shell energy spectrum is emphasized. [1] F. Donati et al., Science 352, 318 (2016). [2] R. Baltic et al., Nano Lett. 16, 7610 (2016). [3] A. B. Shick, D. S. Shapiro, J. Kolorenc, A. I. Lichtenstein, Sci. Rep. 7, 2751 (2017).

CPP 86.5 Fri 11:30 HL 001

Interlayer trions in the MoS$_2$/WS$_2$ van der Waals heterostructure — •Thorsten Deilmann and Kristian Sommer Thygesen — CAMD, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Electronic excitations in van der Waals heterostructures can have interlayer or intralayer character depending on the spatial localisation of the involved charges (electrons and holes). In the case of neutral electron-hole pairs (excitons), both types of excitations have been explored theoretically and experimentally. In contrast, studies of charged trions have so far been limited to the intralayer type.

Here we investigate the complete set of interlayer excitations in a MoS$_2$/WS$_2$ heterostructure using a novel ab-initio method, which allows for a consistent treatment of both excitons and trions at the same theoretical footing. Our calculations predict the existence of bound interlayer trions below the neutral interlayer excitons. We obtain binding energies of 18/28 meV for the positive/negative interlayer trions with both electrons/holes located on the same layer. In contrast, a negligible binding energy is found for trions which have the two equally charged particles on different layers.

CPP 86.6 Fri 11:45 HL 001

The optimal one dimensional periodic table: a modified Pettifor chemical scale from data mining — •Miguel Marques[1] and Antonio Sanna[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck Institut für Microstrukture Physics, Weinberg 2, 06120 Halle, Germany

Starting from the experimental data contained in the inorganic crystal structure database, we use a statistical analysis to determine the likelihood that a chemical element A can be replaced by another B in a given structure. This information can be used to construct a matrix where each entry (A,B) is a measure of this likelihood. By ordering the rows and columns of this matrix in order to reduce its bandwidth, we construct a one-dimension ordering of the chemical elements, analogous to the famous Pettifor scale. The new scale shows large similarities with the one of Pettifor, but also striking differences, especially in what comes to the ordering of the non-metals.

CPP 86.7 Fri 12:00 HL 001

Novel two-dimensional topological insulators from first principles materials screening — •Thomas Olsen and Kristian Thygesen — Technical University of Denmark

We have applied first principles calculations to find new stable two-dimensional materials with non-trivial band topology. The novel materials include more than 10 quantum spin Hall insulators, quantum anomalous Hall insulators and topological crystalline insulators protected by mirror symmetry. We also discuss the dual topological nature of the band structure in the presence of both time-reversal and mirror symmetry and show that odd mirror Chern numbers always imply a quantum spin Hall effect.

CPP 86.8 Fri 12:15 HL 001

Nanoparticles Classification with Self-Organisation Map (SOM) on 3D Electrostatic Potential Surface (EPS) — •Baichuan Sun and Amanda Barnard — Molecular & Materials Modelling, Data61 CSIRO, Door 34 Goods Shed, Village St, Docklands, VIC 3008, Australia

State-of-the-art deep learning (DL) algorithms are having tremendous impact across all scientific fields, and Material Science (MS) is no exception. A combination of computational chemistry simulations and DL techniques requires a hybrid computation/data research workflow, which represents a revolutionary approach to MS studies. There is a gap between the ab initio characterisation of nanomaterials with electronic structure simulations and its analytics with DL frameworks which stems from difficulties in representing quantum mechanical properties in such a way that is suitable for artificial neural networks. To overcome this issue we are evaluating the efficiency of visualising the 3-D Electrostatic Potential Surface (EPS) with Self-organising Maps (SOM), and integrating them directly into reliable DL frameworks. A Self-organisation Map classifies high-dimensional data into low-dimensional (normally 2D) space without supervision, while retaining the intrinsic topological relationship of the data set. As we will show, it is possible to represent a 3D molecular EPS with a single 2D snapshot, or ”fingerprint” of the particle, provided they are orientationally invariant. In this study we demonstrate how Ag nanoparticles 3-D EPS self-organising texture maps can be used to classify nanoparticles based on the energy of the Fermi level.

CPP 86.9 Fri 12:30 HL 001

Regulation of structure and high thermoelectric performance of 1D SnTe via encapsulation within single-walled carbon nanotube — Andrij Vasylenko[1], •Jamie Wynn[2], Sam Marks[1], Paulo V. C. Medeiros[3], Quentin M. Ramasse[4], Andrew J. Morris[4], Jeremy Sloan[1], and David Quigley[1] — [1]University of Warwick, Coventry, UK — [2]University of Cambridge, Cambridge, UK — [3]Daresbury Campus, Darsbury, UK — [4]University of Birmingham, Birmingham, UK

We present the extreme case of nanostructuring, exploiting capillarity of single-walled carbon nanotubes (SWCNTs) for synthesis of the smallest possible thermoelectric SnTe nanowires with cross sections as small as a single atom. By adapting high-throughput ab initio random structure searching, we discover several structures of SnTe that can be formed within SWCNT and compare results with experimentally obtained encapsulated SnTe nanowires. From first principles, we demonstrate that by choosing the appropriate diameter of a template SWCNT, we can manipulate the structure of 1D SnTe and its thermoelectric performance. The demonstrated technique opens a practical route towards nanostructural manipulation of electrical and thermoelectric properties of the 1D materials. The best candidate 1D SnTe structures demonstrate strongly enhanced ZT over a unprecedentedly broad temperature range with a maximum value of 3.25.