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

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Overview of Invited Talks and Sessions

(Lecture halls H8, H13, H14, and H18; Poster B1)

Invited Talks

CPP 1.1	Mon	9:30–10:00	H14	**Building Complex Colloids with Block Copolymers and Topology** — •Andre Groeschel
CPP 1.2	Mon	10:00–10:30	H14	**Gradient dynamics models for films of complex fluids and beyond - Dewetting, line deposition and crystallisation** — •Uwe Thiele
CPP 1.4	Mon	10:45–11:15	H14	**Controlling structure, orientation and nanomorphology in semiconducting and conducting polymer films** — •Martin Brinkmann, Laure Biniek, Vishnu Vijayakumar, Viktoriia Untilova
CPP 1.5	Mon	11:30–12:00	H14	**Conjugated polymers: linking mesoscopic morphology and charge transport** — •Denis Andrienko
CPP 2.1	Mon	9:30–10:00	H18	**The perovskite/transport layer interfaces dominate non-radiative recombination in efficient perovskite solar cells** — •Martin Stolterfoht, Pietro Caprioglio, Christian Wolff, Jose Marquez, Thomas Kirchartz, Thomas Unold, Dieter Neher
CPP 3.1	Mon	9:30–10:00	H13	**Tailoring the Excited State Energy Landscape in Supramolecular Nanostructures** — •Richard Hildner
CPP 9.1	Mon	15:00–15:30	H18	**Bulk Amounts of (6,5) Carbon Nanotubes for (Opto)- Electronic Devices** — •Jana Zaumseil
CPP 20.6	Tue	10:45–11:15	H13	**Dynamic surface tension of soft solids** — Mathijs van Gorcum, Bruno Andreotti, Jacco Snoeijer, •Stefan Karpitschka
CPP 24.1	Tue	10:45–11:15	H14	**Mechanochemical activation of Cu-NHC-complexes : molecular design, force-measurements and application in polymer materials** — •Wolfang H Binder, Michel Biewend, Philipp Michael, Martin Beyer, Matthew Sammon
CPP 24.2	Tue	11:30–12:00	H14	**Mechanoradicals in collagen or: Why playing soccer hurts** — •Frauke Gräter, Christopher Zapp, Agnieszka Obarska-Kosinski, Csaba Daday, Reinhard Kappl
CPP 24.5	Tue	12:30–13:00	H14	**The challenges and opportunities of polymer mechanochemistry** — •Roman Boulatov
CPP 30.1	Wed	9:30–10:00	H14	**Microstructural transitions and characterization of capillary suspensions** — Sebastian Bindgen, Frank Bossler, Irene Natalia, •Erin Koos
CPP 39.1	Wed	15:00–15:30	H14	**Film formation, microstructure and ferroelectricity of MAPbI3 light-harvesting layers** — Holger Röhm, Tobias Leonhard, Alexander Schulz, Susanne Wagner, Michael Hoffmann, •Alexander Colsmann
CPP 39.2	Wed	15:30–16:00	H14	**How do evaporating thin films evolve? Unravelling phase-separation mechanisms during solvent-based fabrication of polymer blends** — •Olga Wodo
CPP 39.7	Wed	17:15–17:45	H14	**Thin film structuring upon liquid-vapor mass exchange** — •Jasper Michels
CPP 48.1	Wed	15:45–16:15	H13	**Many Weak Interactions Make a Difference - from Fuzzy Biomolecular Self Assembly to Superselectivity** — •Ralf Richter
CPP 49.1	Wed	17:15–17:45	H18	**Stimuli-Responsive Polymer-Based Sensors, Muscles, and Drug Delivery Platforms** — •Michael Serpe

CPP 51.1	Thu	9:30–10:00	H13	**Systematic Dynamic Coarse-Graining with Memory** — Gerhard Jung, Martin Hanke, •Friederike Schmid
CPP 56.1	Thu	15:00–15:30	H14	**Microstructure resolved simulations and theory based modeling: Tools for exploring the inner life of a battery** — •Arnulf Latz
CPP 56.3	Thu	15:45–16:15	H14	**Increasing the rate capability of thick graphite electrodes: Insights from MRI, NMR and porous electrode theory modelling** — •Jamie Foster
CPP 56.5	Thu	16:45–17:15	H14	**Numerical Simulation and Machine Learning in Virtual Materials Design** — •Jan Hamaekers
CPP 58.1	Thu	15:00–15:30	H13	**Gyroids on the nanoscale: Metamaterials with surprising optical properties** — •Bodo Wilts
CPP 59.1	Thu	15:00–15:30	H8	**Polymer-Grafted Nanoparticle Membranes with Exceptional Gas Separation Performance** — •Sanat Kumar
CPP 66.1	Fri	9:45–10:15	H18	**Coupled Organic-Inorganic Nanostructures for Optical Switches** — •Marcus Scheele

Invited talks of the joint Symposium SKM Dissertation-Prize 2019

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:50	H2	**Synchronization and Waves in Confined Complex Active Media** — •Jan Frederik Totz
SYSD 1.2	Mon	9:50–10:10	H2	**Spin scattering of topologically protected electrons at defects** — •Philipp Rüssmann
SYSD 1.3	Mon	10:10–10:30	H2	**Beyond the molecular movie: Revealing the microscopic processes behind photo-induced phase transitions** — •Chris W. Nicholson
SYSD 1.4	Mon	10:30–10:50	H2	**Thermodynamic bounds on current fluctuations** — •Patrick Pietzonka
SYSD 1.5	Mon	10:50–11:10	H2	**Lightwave-driven quasiparticle acceleration** — •Fabian Langer
SYSD 1.6	Mon	11:10–11:30	H2	**Ultrafast plasmon-driven point-projection electron microscopy** — •Jan Vogelsang
SYSD 1.7	Mon	11:30–11:50	H2	**Helimagnets, sand patterns and fingerprints linked by topology** — •Peggy Schönherr

Invited talks of the joint Symposium Mechanically Controlled Electrical Conductivity of Oxides

See SYCO for the full program of the symposium.

SYCO 1.1	Mon	9:30–10:00	H1	**Dislocation Dynamics and Their Conductivities in Oxides** — •Yuichi Ikuhara
SYCO 1.2	Mon	10:00–10:30	H1	**Strain effects in ionic conductivity and electrode processes** — •Jürgen Janek
SYCO 1.3	Mon	10:30–11:00	H1	**Elastic dipoles of point defects in materials** — •Celine Varvenne
SYCO 1.4	Mon	11:30–12:00	H1	**Mapping strain/pressure with ZnO nanowire arrays by piezo-phototronic effect** — •Caofeng Pan
SYCO 1.5	Mon	12:00–12:30	H1	**Bulk and Flexo-photovoltaic effect** — •Marin Alexe

Invited talks of the joint Symposium Patterns in Nature: Origins, Universality, Functions

See SYPN for the full program of the symposium.

SYPN 1.1	Mon	15:00–15:30	H1	**Engineering spatial-temporal organization of bacterial suspensions** — •Igor Aronson
SYPN 1.2	Mon	15:30–16:00	H1	**Collective behaviour and pattern formation in phoretic active matter** — •Ramin Golestanian
SYPN 1.3	Mon	16:00–16:30	H1	**Control and selection of spatio-temporal patterns in complex systems** — •Svetlana Gurevich
SYPN 1.4	Mon	16:45–17:15	H1	**Self-organization of Active Surfaces** — •Frank Jülicher
SYPN 1.5	Mon	17:15–17:45	H1	**Front instabilities can reverse desertification** — •Ehud Meron

Invited talks of the joint Symposium Czech Republic as Guest of Honor

See SYCZ for the full program of the symposium.

SYCZ 1.1	Thu	9:30–10:00	H4	**Crystal symmetries and transport phenomena in antiferromagnets** — •Tomas Jungwirth
SYCZ 1.2	Thu	10:00–10:30	H4	**Terahertz subcycle charge and spin control** — •Rupert Huber
SYCZ 1.3	Thu	10:30–11:00	H4	**1D molecular system on surfaces** — •Pavel Jelinek
SYCZ 1.4	Thu	11:15–11:45	H4	**Tunneling microscopy on insulators provides access to out-of-equilibrium charge states** — •Jascha Repp
SYCZ 1.5	Thu	11:45–12:15	H4	**Occam's razor and complex networks from brain to climate** — •Jaroslav Hlinka
SYCZ 1.6	Thu	12:15–12:45	H4	**Long range temporal correlations in complex systems** — •Holger Kantz

Invited talks of the joint Symposium Physics of Self-Organization in DNA Nanostructures

See SYDN for the full program of the symposium.

SYDN 1.1	Thu	9:30–10:00	H1	**Functional DNA Nanostructures and Their Applications** — •Itamar Willner
SYDN 1.2	Thu	10:00–10:30	H1	**Gaining control of DNA-based nanodevices** — •Francesco Ricci
SYDN 1.3	Thu	10:30–11:00	H1	**Self-assembly and optical properties of single molecule polymers on DNA origami** — •Kurt Gothelf
SYDN 1.4	Thu	11:15–11:45	H1	**DNA origami route to dynamic plasmonics** — •Laura Liu
SYDN 1.5	Thu	11:45–12:15	H1	**DNA templated metal nanostructures** — •Ralf Seidel

Sessions

CPP 1.1–1.7	Mon	9:30–12:30	H14	**Focus: Morphology of Complex Polymer Mesophases: From Experiment to Modelling - organized by Kostas Daoulas and Volker Abetz**
CPP 2.1–2.11	Mon	9:30–12:45	H18	**Hybrid and Perovskite Photovoltaics I**
CPP 3.1–3.12	Mon	9:30–13:00	H13	**Molecular Electronics and Excited State Properties**
CPP 4.1–4.10	Mon	9:30–12:15	H8	**Responsive and Adaptive Systems (joint session CPP/DY)**
CPP 5.1–5.9	Mon	9:30–12:30	H10	**Membranes and vesicles I (joint session BP/CPP)**
CPP 6.1–6.11	Mon	9:30–12:45	H20	**Active Matter A (joint session DY/CPP)**
CPP 7.1–7.9	Mon	10:30–13:00	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge I (joint session O/TT/CPP/DS)**
CPP 8.1–8.8	Mon	15:00–17:15	H14	**Interfaces and Thin Films (joint session CPP/DY)**
CPP 9.1–9.7	Mon	15:00–17:15	H18	**Organic Electronics and Photovoltaics I - Charge Transport and Electronic Devices**
CPP 10.1–10.9	Mon	15:00–17:30	H13	**Crystallization, Nucleation and Self-assembly I**
CPP 11.1–11.4	Mon	15:00–16:00	H8	**Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods**
CPP 12.1–12.10	Mon	15:00–17:30	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge II (joint session O/TT/DS/CPP)**
CPP 13.1–13.5	Mon	15:00–16:15	H10	**Membranes and Vesicles II (joint session BP/CPP)**
CPP 14.1–14.8	Mon	15:00–17:15	H31	**Organic photovoltaics and electronics (joint session HL/CPP)**
CPP 15.1–15.7	Mon	15:45–18:30	H46	**Symposium SYCO of the divisions MM (leading), O, CPP, KFM and DS continued as topical session: Mechanically controlled electrical conductivity of oxides (joint session MM/CPP/O)**
CPP 16.1–16.5	Mon	16:15–17:30	H8	**Glasses and Glass Transition (joint session CPP/DY)**
CPP 17.1–17.44	Mon	17:30–19:30	Poster B1	**Poster Session I**
CPP 18.1–18.4	Tue	9:30–10:30	H14	**Crystallization, Nucleation and Self-Assembly II (joint session CPP/BP)**
CPP 19.1–19.11	Tue	9:30–12:30	H18	**Hybrid and Perovskite Photovoltaics II**
CPP 20.1–20.12	Tue	9:30–13:00	H13	**Wetting, Fluidics and Liquids at Interfaces and Surfaces (joint session CPP/DY)**
CPP 21.1–21.13	Tue	9:30–13:00	H36	**Two-dimensional Materials I (joint session HL/CPP)**

CPP 22.1–22.9	Tue	10:30–12:45	H8	**Plasmonics I (joint session O/CPP)**
CPP 23.1–23.9	Tue	10:30–13:00	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge III (joint session O/CPP/DS/TT)**
CPP 24.1–24.5	Tue	10:45–13:00	H14	**Focus: Mechanoresponsive Molecules and Materials - organized by Kerstin Blank and Robert Göstl**
CPP 25.1–25.58	Tue	14:00–16:00	Poster B1	**Poster Session II**
CPP 26.1–26.7	Tue	14:00–15:45	H3	**Active Matter B (joint session DY/CPP)**
CPP 27.1–27.10	Tue	14:00–16:30	H8	**Plasmonics II (joint session O/CPP)**
CPP 28.1–28.10	Tue	14:00–16:45	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge IV (joint session O/CPP/DS/TT)**
CPP 29.1–29.7	Tue	14:00–15:45	H36	**Two-dimensional Materials II: graphene (joint session HL/CPP)**
CPP 30.1–30.11	Wed	9:30–12:45	H14	**Complex Fluids and Colloids, Micelles and Vesicles (joint session CPP/DY)**
CPP 31.1–31.6	Wed	9:30–11:00	H18	**Organic Electronics and Photovoltaics II - Non-Fullerene Organic Solar Cells**
CPP 32.1–32.13	Wed	9:30–13:00	H13	**Charged Soft Matter, Polyelectrolytes and Ionic Liquids I**
CPP 33.1–33.12	Wed	9:30–13:00	H4	**Active Matter I (joint session BP/CPP/DY)**
CPP 34.1–34.13	Wed	9:30–13:00	H36	**Two-dimensional Materials III (joint session HL/CPP)**
CPP 35.1–35.11	Wed	10:30–13:15	H8	**Plasmonics III (joint session O/CPP)**
CPP 36.1–36.9	Wed	10:30–13:15	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge V (joint session O/CPP/DS/TT)**
CPP 37.1–37.55	Wed	11:00–13:00	Poster B1	**Poster Session III**
CPP 38.1–38.5	Wed	11:30–12:45	H18	**Polymer Networks and Elastomers**
CPP 39.1–39.11	Wed	15:00–18:45	H14	**Focus: Controlling Phase Formation Dynamics in Solution Processed Semiconductors - organized by Christoph Brabec, Jens Harting and Hans-Joachim Egelhaaf**
CPP 40.1–40.8	Wed	15:00–17:00	H18	**Modeling and Simulation of Soft Matter I (joint session CPP/DY)**
CPP 41.1–41.2	Wed	15:00–15:30	H13	**Charged Soft Matter, Polyelectrolytes and Ionic Liquids II**
CPP 42.1–42.11	Wed	15:00–17:45	H8	**Plasmonics IV (joint session O/CPP)**
CPP 43.1–43.11	Wed	15:00–17:45	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge VI (joint session O/DS/CPP/TT)**
CPP 44.1–44.13	Wed	15:00–18:45	H20	**Condensed-matter simulations augmented by advanced statistical methodologies (joint session DY/CPP)**
CPP 45.1–45.9	Wed	15:00–17:30	H36	**Photovoltaics (joint session HL/CPP)**
CPP 46.1–46.9	Wed	15:30–18:00	H19	**Microswimmers (joint session DY/CPP)**
CPP 47.1–47.15	Wed	15:00–19:15	H3	**Complex Fluids and Soft Matter (joint session DY/CPP)**
CPP 48.1–48.9	Wed	15:45–18:30	H13	**Biopolymers, Biomaterials and Bioinspired Functional Materials (joint session CPP/BP)**
CPP 49.1–49.4	Wed	17:15–18:30	H18	**Hydrogel und Microgel**
CPP 50.1–50.13	Thu	9:30–13:00	H18	**Organic Electronics and Photovoltaics III - Organic Photovoltaics**
CPP 51.1–51.8	Thu	9:30–12:00	H13	**Modeling and Simulation of Soft Matter II (joint session CPP/DY)**
CPP 52.1–52.12	Thu	9:30–12:45	H10	**Biomaterials and biopolymers I (joint session BP/CPP)**
CPP 53.1–53.13	Thu	9:30–13:00	H36	**Perovskite and Hybrid Photovolatics I (joint session HL/CPP)**
CPP 54.1–54.10	Thu	10:00–12:45	H19	**Active Matter II (joint session DY/CPP)**
CPP 55.1–55.3	Thu	12:15–13:00	H13	**Physics of Self-Organization in DNA Nanostructures (joint session CPP/BP)**
CPP 56.1–56.8	Thu	15:00–18:00	H14	**Focus: Computational Methods for the Energy Transition: Paving the Road to Future Materials and Storage Systems - organized by Stephan Kramer and Jochen Zausch**
CPP 57.1–57.12	Thu	15:00–18:15	H18	**Organic Electronics and Photovoltaics IV - Excitonic Properties and Light-Emitting Devices**
CPP 58.1–58.12	Thu	15:00–18:30	H13	**Nanostructures, Nanostructuring and Nanosized Soft Matter**
CPP 59.1–59.8	Thu	15:00–17:30	H8	**Composites and Functional Polymer Hybrids**
CPP 60.1–60.7	Thu	15:00–17:00	H10	**Biomaterials and biopolymers II (joint session BP/CPP)**

CPP 61.1–61.9	Thu	15:00–17:30	H36	**Perovskite and Hybrid Photovolatics II (joint session HL/CPP)**
CPP 62.1–62.3	Thu	17:45–18:30	H8	**Electrical, Dielectrical and Optical Properties of Thin Films**
CPP 63	Thu	18:45–19:45	H13	**Annual General Meeting of the CPP Division (CPP Mitgliederversammlung)**
CPP 64.1–64.10	Fri	9:30–12:00	H11	**Active Matter III (joint session BP/CPP/DY)**
CPP 65.1–65.13	Fri	9:30–13:00	H36	**Two-dimensional Materials IV (joint session HL/CPP)**
CPP 66.1–66.7	Fri	9:45–12:00	H18	**Organic Electronics and Photovoltaics V - Semiconducting Properties and Devices**
CPP 67.1–67.9	Fri	9:45–12:15	H13	**Polymer and Molecular Dynamics, Friction and Rheology**
CPP 68.1–68.8	Fri	10:00–12:15	H6	**Microfluidics (joint session DY/CPP)**
CPP 69.1–69.7	Fri	10:00–11:45	H19	**Glasses and Glass transition (joint session DY/CPP)**
CPP 70.1–70.1	Fri	12:30–13:15	H1	**Closing talk (joint session BP/CPP/DY)**

Annual General Meeting of the Chemical and Polymer Physics Division

Thursday 18:45–19:45 H13

- Report of the current speaker team
- Election of the second deputy speaker
- Award of the poster prizes of the CPP Division
- Miscellaneous

CPP 1: Focus: Morphology of Complex Polymer Mesophases: From Experiment to Modelling - organized by Kostas Daoulas and Volker Abetz

Time: Monday 9:30–12:30 Location: H14

Invited Talk CPP 1.1 Mon 9:30 H14
Building Complex Colloids with Block Copolymers and Topology — •Andre Groeschel — Physical Chemistry and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg Essen, 47057 Duisburg, Germany

Colloids are omnipresent in nature as well as our everyday lives, e.g. in paint, milk, as quantum dots or colloidal gold. For technological applications colloids are typically synthesized using equipment or wet chemical processes giving access to particles of well-controlled sizes. In nature however, biological colloids are often self-assembled from smaller building blocks. Virus particles are composed of a defined number of proteins, giving viruses a complex composition, surface chemistry, and in some cases, also shape-anisotropy on length scales as small as 20 nm. Inspired by the natural structuring abilities, self-assembly concepts are now researched that allow the synthesis of colloids with comparable level of detail and control.

This presentation summarizes our efforts to create complex colloids using concepts of self-assembly, block copolymers and topology. Block copolymers are comparably primitive but versatile building blocks that are able to assemble into microparticles with unusual shapes, mesoscopic inner structure, and functional 2D/3D surfaces. To better understand the relationship between topology an mesostructure, we analyze the particles with electron tomography and resolve the delicate 3D arrangement of polymer domains through reconstructions.

Invited Talk CPP 1.2 Mon 10:00 H14
Gradient dynamics models for films of complex fluids and beyond - Dewetting, line deposition and crystallisation — •Uwe Thiele — Institut für Theoretische Physik and Center for Nonlinear Science, Universität Münster.

First, we review situations where the dynamics of phase transitions creates structures, e.g., dewetting polymer mixtures, Langmuir-Blodgett (LB) transfer of surfactants or colloidal crystallisation. After presenting typical hydrodynamic thin-film models we rewrite them as gradient dynamics on some energy functional that accounts for wettability and capillarity. This allows for many consistent extensions, e.g., towards solute-dependent wettability. As example we show that a film of a mixture may become unstable through coupled film height and concentration fluctuations. Next, we consider gradient dynamics models for films covered by surfactants. Such models may be employed to describe the formation of line patterns during LB transfer of a surfactant layer from a bath onto a moving plate. After showing simulations with the full model, we sketch how line deposition is reflected in an intricate bifurcation structure that one can analyse within a Cahn-Hilliard-type model. Finally, we consider colloidal crystallisation employing gradient dynamics models, namely, dynamical density functional theory (DDFT) and its local approximation, the phase field crystal (PFC) model. We analyse crystallisation fronts and show that their speeds may be obtained via a marginal stability criterion and relate it to created disorder and subsequent aging. Finally, we discuss the relation of localised states and an amorphous solid phase.

CPP 1.3 Mon 10:30 H14
Optimum Disorder of Polymer Mesoparticle Aggregates for Efficient Thermal Insulation — Fabian Nutz[1], Alexandra Philipp[1], Bernd Kopera[1], Martin Dulle[2], and •Markus Retsch[1] — [1]Physical Chemistry I, University of Bayreuth, 95447 Bayreuth, Germany — [2]JCNS-1/ICS-1: Neutron Scattering Forschungszentrum, Juelich, Germany

Heat transport plays a critical role in modern batteries, electrodes, and capacitors. This is caused by the ongoing miniaturization of such nano-technological devices, which increases the local power density and hence temperature. Even worse, the introduction of heterostructures and interfaces is often accompanied by a reduction in thermal conductivity, which can ultimately lead to the failure of the entire device. Surprisingly, a fundamental understanding of the governing heat transport processes even in simple systems is still missing. This contribution closes this gap and elucidates how strongly the morphology of a model particulate system influences the effective thermal conductivity across such a complex mesostructure. In a combined experimental and modeling approach, well-defined mixtures of monodisperse particles with varying size ratios were investigated. The transition from order to disorder can reduce the effective thermal conductivity by as much as ~50%. This is caused by an increase in the thermal transport path length and is governed by the number of inter-particle contact points.

Invited Talk CPP 1.4 Mon 10:45 H14
Controlling structure, orientation and nanomorphology in semi-conducting and conducting polymer films — •Martin Brinkmann, Laure Biniek, Vishnu Vijayakumar, and Viktoriia Untilova — Université de Strasbourg, Institut Charles Sadron, CNRS, Strasbourg, France

Conducting and semi-conducting polymers are omnipresent in plastic electronics nowadays. Although structure-property correlations are central for device optimization, there is still insufficient understanding of the mechanisms and principles that govern thin film growth and chain packing, especially for the recent low band gap polymers of increasing molecular complexity e.g. p(NDIT2OD), PTB7, PCE11 and PCPDTBT. Crystallization/orientation of polymer semiconductors using epitaxy or high temperature rubbing is an elegant manner to tune their structure and organization that can further be investigated by transmission electron microscopy at different length scales. This contribution summarizes recent efforts of our group in this context and shows how the progress in mastering crystallization/orientation of semi-conducting polymers can be transposed to their conducting counterparts after soft doping. We demonstrate the possibility to fabricate highly oriented conducting polymer films whose charge conductivity and thermopower can reach beyond that of iodine-doped polyacetylene.

15 min. break

Invited Talk CPP 1.5 Mon 11:30 H14
Conjugated polymers: linking mesoscopic morphology and charge transport — •Denis Andrienko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We first discuss the complex relation between processing, polymorphism, and structure formation in several conjugated polymers: P3HT,[1] PCPDTBT,[2] and PBTTT.[3] Their mesoscopic morphology, as elucidated by combining various experimental and atomistic simulation techniques, is used to explain particular features of charge carrier mobility.[6] We then assess various strategies for in silico prediction of morphologies and electronic properties of conjugated polymers, starting solely from the chemical structure.[4,5] Though it is too optimistic to say that we are approaching a true bottom-up multiscale modeling of conjugated polymers, the benefits from using computer simulations to complement experimental results are obvious.

[1] C. Poelking, D. Andrienko, Macromolecules, 46, 8941, 2013.

[2] F. Fischer, G. Schulz, D. Trefz, A. Melnyk, M. Brinkmann, D. Andrienko, S. Ludwigs, Macromolecules, 50, 1402, 2017.

[3] A. Melnyk, M. Junk, M. McGehee, B. Chmelka, M. R. Hansen, D. Andrienko, J. Phys. Chem. Lett., 8, 4155, 2017.

[4] C. Scherer, D. Andrienko, Eur. Phys. J. Spec. Top., 225, 1441, 2016.

[5] P. Gemuenden, C. Poelking, K. Kremer, K. Daoulas, D. Andrienko, Macromol. Rapid Commun., 36, 1047, 2015.

[6] Sh. Ye, L. Janasz, W. Zajaczkowski, J. G. Manion, A. Mondal, T. Marszalek, D. Andrienko, K. Muellen, W. Pisula, D. S. Seferos, Macromol. Rapid Commun., 1800596, 2018

CPP 1.6 Mon 12:00 H14
Engineering scale simulation of non-equilibrium network phases for battery electrolytes — •Ludwig Schneider and Marcus Mueller — Georg-August Universität Göttingen, Institute for Theoretical Physics, Göttingen, Germany

Diblock copolymer materials exhibit a rich equilibrium phase diagram, qualifying them for applications in fuel cells, filters, and battery materials. Self-assembly of these materials rarely results in the equilibrium structures. Instead, configurations are trapped in long-lived metastable states and can be stabilized via cross-linking or cooling below the glass transition temperature of one component. The properties of these structures, such as ion-conductivity, can deviate from those of corresponding equilibrium phases.

SOMA, our massively-parallel implementation of the Single-Chain-in-Mean-Field (SCMF) algorithm, enables us to study systems with billions of particles and predict their structure formation, thus unraveling the transport properties of self-assembled diblock-copolymers as a function of volume fraction, f. Our investigations show that non-equilibrium morphologies exhibit a large scale fractal-like domain structure that influences the transport properties. The length scale of these structures highlight the necessity of large system sizes to obtain bulk properties. We quantify the transport via the tortuosity and the diffusion inside the network phase and show that equilibrium phases overestimate the transport capabilities of random networks.

CPP 1.7 Mon 12:15 H14

Multiscale modelling of multidimensional molecular architectures for efficient organic solar cells — Marvin Nyenhuis, •Marcus Böckmann, and Nikos Doltsinis — Institut für Festkörpertheorie, Westfälische Wilhems-Universität, Münster, Germany

The active layer of bulk hetero-junction (BHJ) organic solar cells (OSCs) constitutes a complex mixture of polymeric donor (D) and acceptor (A) compounds [1] and its morphology is known to change upon *ad hoc* thermal annealing, thereby increasing the overall photoconversion efficiency (PCE). While experimental techniques like STM or AFM yield but detailed information of the surface structure, we use multidimensional Molecular Dynamics simulations [2] to elucidate the interior constitution of the layer at the atomistic level. In this contribution, we present insight obtained recently for the interpretation of morphology related UV-vis spectra and domain formation [3,4] together with current results on a novel polymeric D/A mixture [5].

[1] A. J. Heeger, Adv. Mater. 2014, 26, 10. [2] M. Böckmann, D. Marx, C. Peter, L. Delle Site, K. Kremer, and N. Doltsinis, Phys. Chem. Chem. Phys. 2011, 10, 1039. [3] M. Böckmann, T. Schemme, D. de Jong, C. Denz, A. Heuer, and N. Doltsinis, Phys. Chem. Chem. Phys. 2015, 17, 28616. [4] T. Winands, M. Böckmann, T. Schemme, P. Ly, D. de Jong, Z. Wang, C. Denz, A. Heuer, and N. Doltsinis, Phys. Chem. Chem. Phys. 2016, 18, 6217. [5] D. Meng, H. Fu, C. Xiao, X. Meng, T. Winands, W. Ma, W. Wei, B. Fan, L. Huo, N. Doltsinis, Y. Li, Y. Sun, and Z. Wang, J. Am. Chem. Soc. 2016, 138, 10184.

CPP 2: Hybrid and Perovskite Photovoltaics I

Time: Monday 9:30–12:45 Location: H18

Invited Talk CPP 2.1 Mon 9:30 H18

The perovskite/transport layer interfaces dominate non-radiative recombination in efficient perovskite solar cells — •Martin Stolterfoht[1], Pietro Caprioglio[1], Christian Wolff[1], Jose Marquez[2], Thomas Kirchartz[3], Thomas Unold[2], and Dieter Neher[1] — [1]University of Potsdam — [2]Helmholtz-Zentrum-Berlin — [3]Forschungszentrum Jülich

Charge transport layers (CTLs) are key components of diffusion controlled perovskite solar cells, however they can induce additional non-radiative recombination pathways. By measuring the quasi-Fermi level splitting (QFLS) of perovskite/CTL heterojunctions, we quantify the interfacial recombination current for a wide range of commonly used CTLs, including various hole-transporting polymers, spiro-OMeTAD, metal oxides and fullerenes. We find that all studied CTLs limit the open-circuit voltage (Voc) by inducing a recombination current that is significantly larger than the loss in the neat perovskite and that the least-selective interface sets the upper limit for the device Voc. The results also show that the Voc equals the internal QFLS in the absorber layer of pin and nip-type cells with selective CTLs and power conversion efficiencies of up to 21.4% (in pin). However, in case of less selective CTLs, the Voc is substantially lower than the QFLS which indicates additional losses at the contacts and/or interfaces. The findings are corroborated by rigorous device simulations which outline several important considerations to maximize the Voc. This work shows that the real challenge to approach the radiative Voc limit lies in the suppression of carrier recombination at the perovskite/CTL interfaces.

CPP 2.2 Mon 10:00 H18

The interplay of interfacial charges, contact layers and hysteresis in perovskite solar cells — Ilka M Hermes[1], Yi Hou[2], Christoph Brabec[2], and •Stefan A.L. Weber[1,3] — [1]MPI for Polymer Research Mainz, Germany — [2]Institute of Materials for Electronics and Energy Technology, Friedrich-Alexander University Erlangen-Nürnberg, Germany — [3]Institute of Physics, Johannes Gutenberg University Mainz, Germany

The charge selective contact layers in perovskite solar cells affect device properties such as current density-voltage hysteresis. Using fullerene-based electron transport layers (ETLs), hysteresis could be suppressed by a reduction of the mobile ion concentration. However, the effect the ETL on the electronic properties of other constituent device layers remains unclear. Using Kelvin probe force microscopy, we compared potential distributions of methylammonium lead iodide-based solar cells with different ETLs, such as planar titania and a C60-derivative, with vastly different hysteretic behavior. We found the most significant potential differences at the interface to the organic hole transport layer spiroMeOTAD. Our results show that the choice of ETL not only influences the extraction and recombination at the perovskite/ETL interface but also changes the transport properties of the spiroMeOTAD layer. We propose that the higher density of mobile ions in the titania cell caused a reaction between iodide anions with the p-doped spiroMeOTAD to form a neutral interface layer, which increased the interfacial resistance and capacitance at the spiroMeOTAD interface.

CPP 2.3 Mon 10:15 H18

Investigation of Charge Transport Properties of cross-linkable Hole Transport Materials in Perovskite Solar Cell Devices — •Simon Ewertowski[1], Lorena Perdigón Toro[2], Dieter Neher[2], and Klaus Meerholz[1] — [1]University of Cologne, Institute of Physical Chemistry, Cologne, Germany — [2]University of Potsdam, Institute of Physics, Potsdam, Germany

Organic-inorganic hybrid perovskite materials are known to show impressive properties in charge generation and charge transport. These properties make them useful in optoelectronic thin film devices, such as light emitting diodes or solar cells. Therefore, perovskite solar cells (PSCs) attracted much attention in the last decade due to their rapid evolution in power conversion efficiencies (PCE), today exceeding 20%.[1] In the inverted p-i-n structured PSCs usually PEDOT:PSS, PTAA and poly TPD are used as efficient hole transport materials (HTMs).[2],[3]

In this study, several oxetane-functionalized cross-linkable x-HTMs such as QUPD[4] are implemented in lead based PSCs. Impedance measurements reveal information about the charge transport across the interfaces between the x-HTMs and the perovskite. These results are taken into account, when analyzing the respective current-voltage characteristics of the built solar cells.

[1] Brenner, T. M. et al., Nat. Rev. Mater. 2016, 1, 15007 [2] Zhao D. et al., Adv. Energy Mater. 2014, 1401855 [3] Wolff C. M. et al., Adv. Mater. 2017, 29, 1700159 [4] Jhuo H.-J., et al., J. Mater. Chem. A, 2015, 3, 9291

CPP 2.4 Mon 10:30 H18

Probing Charge Carrier Dynamics in Perovskite Solar Cells — •Christian Wolff[1], Sean Bourelle[2], Sascha Feldmann[2], Felix Deschler[2], and Dieter Neher[1] — [1]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, Potsdam, Germany — [2]Cavendish Laboratory, Department of Physics, University of Cambridge, JJ Thomson Ave., Cambridge, UK

Photogenerated charge carriers in solar cells have different pathways of recombining. The ideal pathway is external recombination while delivering power to a consumer. In parallel charge carriers may recombine radiatively or nonradiatively in the bulk of the absorber, at surface states, within other functional layers, or across internal interfaces. One major challenge in solar cell research is to identify the pathway, order and rate of these processes. In this contribution we probe the fate of charge carriers in fully functioning devices. We employ time-resolved and steady state absorption, luminescence and charge extraction experiments and provide a consistent picture of the dominating recombination processes at relevant carrier densities. We are able to show that the recombination under 1 sun illumination is dominated by a first order process that we attribute to interfacial recombination, while at higher intensities a radiative second order is prevailing. The results suggest that unlike other previous reports the recombination process in full devices follows the simple rate equation $dn/dt = -k_1 n + k_2 n^2 + k_3 n^3$, with $k_1 \sim 10^7 s^{-1}$, $k_2 \sim 10^{-11} cm^{-3} s^{-1}$ and $k_3 \sim 10^{-33} cm^{-6} s^{-1}$ and that there is no need to include mixed-order processes.

CPP 2.5 Mon 10:45 H18

Universal self-assembled monolayers as hole contacts for high-performance p-i-n Perovskite solar cells — •Amran Al-Ashouri[1], Artiom Magomedov[2], Marcel Ross[1], José M. Prieto[1], Eike Köhnen[1], Marko Jošt[1], Tadas Malinauskas[2], Thomas Unold[1], Vytautas Getautis[2], and Steve Albrecht[1] — [1]HZB, Berlin, Germany — [2]KTU, Kaunas, Lithuania

We recently presented a novel concept for hole-selective contacts in perovskite solar cells (PSCs) by utilizing a molecule that forms a self-assembled monolayer (SAM) on the transparent conductive oxide via covalent bonds [1]. Here we present results from a new class of hole-selective SAMs that enable p-i-n PSCs with open-circuit voltages (Voc's) of up to 1.19 V, fill factors of over 80 % and thus power conversion efficiencies of up to 21 % for three different perovskite compositions. Hyperspectral, absolute and transient photoluminescence spectroscopy reveal that the reduction of non-radiative recombination losses at the hole contact interface, accompanied by high charge carrier lifetimes, is partially the origin of the relatively high Voc. Interestingly, implementing the SAMs also reduces non-radiative recombination at the electron-selective contact (C60). We further analyze the SAMs by IR and X-ray spectroscopy to assess the surface modification and energetic alignments. Our work demonstrates cell performances that rival best published p-i-n PSCs, without any interlayers, doping or perovskite post-treatments and might therefore serve as a suitable strategy for further performance improvements.

[1] Magomedov et al. *Adv. Energy Mater.* 2018, **8**, 1801892

CPP 2.6 Mon 11:00 H18

Interfacial Characteristics and Charge Carrier Dynamics in Formamidinium Tin Iodide and Phenylethylammonium/Formamidinium Tin Iodide — •Jonas Horn[1], Mirko Scholz[2], Kawon Oum[2], Thomas Lenzer[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik — [2]Universität Siegen, Physikalische Chemie

Electrical and optical measurements were performed at formamidinium tin iodide ($FASnI_3$) and its phenylethylammonium (PEA) derivative $PEA_{0.08}FA_{0.92}SnI_3$, representing attractive alternatives to lead-based perovskites. Charge transport across metal-perovskite interfaces and through the perovskite films were studied on microstructured gold electrode arrays. Hysteresis in the current-voltage characteristics and a corresponding current-time behavior indicated limitation by interfacial charge transfer. Smaller persistent changes following prolonged polarization was measured in $PEA_{0.08}FA_{0.92}SnI_3$ compared to $FASnI_3$ which is explained by a 2-dimensional interlayer at the contacts leading to decreased field-induced migration of ions. The rate constants for the Auger- and bimolecular recombination processes were obtained from femtosecond transient absorption experiments. A time constant of 0.5 ps was found for the scattering of charge carriers by optical phonons, even faster than measured in lead-based perovskites. Carrier recombination in the bulk material was not substantially influenced by the substitution of FA by PEA. Changes in the electrical characteristics of $PEA_{0.08}FA_{0.92}SnI_3$ compared to $FASnI_3$ are, therefore, assigned to different contact rather than bulk characteristics.

15 min. break

CPP 2.7 Mon 11:30 H18

Quantitative Analysis of the Transient Photoluminescence of Lead Halide Perovskite with Contact Layers — •Benedikt Krogmeier[1], Lisa Krückemeier[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

Transient photoluminescence (PL) is a powerful measurement technique to study charge carrier dynamics in perovskite layers. A single layer of lead halide perovskite measured with this technique usually shows a high charge carrier lifetime. However, adding additional contact layers may substantially accelerate the PL decay and therefore decrease the measured lifetime. The higher decay occurs due to the extraction of charge carriers into the contact layer or due to charge carrier recombination at the interface. As the measurements are done on uncontacted samples (i.e. in open circuit), charge carriers may accumulate on the contacts after extraction and thereby repel additional charges at longer times and higher laser fluences. The superposition of extraction, accumulation and recombination makes the use of numerical simulations necessary. We use these simulations to describe experimental results on various structures featuring, zero, one or two contact layers. In addition, we study the effect of low conductivity interface layers (such as PTAA or PCBM) and the effect of high conductivity layers such as indium tin oxide or silver on lateral diffusion and thereby the decay kinetics.

CPP 2.8 Mon 11:45 H18

Charge carrier recombination dynamics and carrier-phonon interactions in bismuth halide semiconductors — •Lissa Eyre, Robert Hoye, Tudor Thomas, Hannah Joyce, and Felix Deschler — University of Cambridge, JJ Thomson Ave, Cambridge, CB3 0HE, United Kingdom

A promising class of lead-free perovskites for photovoltaic applications include the bismuth halides, such as MA3Bi2I9, BiOI, and Cs2AgBiBr6. Although these materials have been predicted to exhibit defect tolerance, as seen in lead-halide perovskites, and already display improved stabilities and long charge carrier lifetimes, the power conversion efficiencies of the corresponding devices have not reached the level of lead-based perovskites. Potential reasons for this are explored, for example, the disconnected nature of the bismuth halide octahedra in the crystal structure, which limits carrier mobility, and the lower levels of absorption due to indirect bandgaps. We probe the behaviour of excited states in many bismuth-halide compounds with various effective dimensionalities using ultrafast transient absorption, Raman, and teraherz spectroscopy. Overall, this work indicates that bismuth-based materials have the potential to be used in efficient optoelectronic devices, but there is a need to account for the effects of strong carrier-phonon coupling and localisation of electronic states on carrier scattering rates. We therefore present charge carrier-lattice interaction strength as an important design criterion for efficient next-generation solar cells.

CPP 2.9 Mon 12:00 H18

Origin of Efficient Photoluminescence in Alloyed Perovskites: Photodoping from Localized Charge Accumulation Regions — •Sascha Feldmann[1], Stuart Macpherson[1], Jasmine Rivett[1], Mojtaba Abdi-Jalebi[1], Guangjun Nan[2], Gregory Tainter[1], Richard Friend[1], Henning Sirringhaus[1], Michael Saliba[3], David Beljonne[4], Samuel Stranks[1], and Felix Deschler[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]Department of Physics, Zhejiang Normal University, Jinhua 321004, China — [3]Adolphe Merkle Institute, University of Fribourg, CH-1700 Fribourg, Switzerland — [4]Chimie des Matériaux Nouveaux, Université de Mons, B-7000 Mons, Belgium

Metal-halide perovskites have emerged as exceptional semiconductors for optoelectronic applications. Here, we reveal the origin of the improved optoelectronic performance arising from compositional engineering by tracking charge carrier dynamics in alloyed perovskites with time-resolved spectroscopy. In contrast to single-halide perovskites, we find that luminescence yields show weak dependence on carrier density and remain high even for photo-excited carrier densities far below solar illumination conditions. We show that the carrier recombination regime changes from second to first order within the first tens of nanoseconds after excitation. Supported by evidence of microscale variations in optical bandgap, electrically-gated transport measurements and first-principles calculations, we propose that spatially-varying energetic disorder in the electronic states leads to local accumulation of one charge carrier type, creating photodoped p- and n-type regions.

CPP 2.10 Mon 12:15 H18

Charge Carrier Transport in Organo-Metal Halide Perovskites Probed by Transient Microwave Conductivity — •Andreas Baumann[1], Manuel Ullrich[2], Nathania Henning[2], Patrick Dörflinger[2], Vladimir Dyakonov[2], and Andreas Sperlich[2] — [1]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg — [2]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

The charge carrier mobility is one of the important intrinsic parameters for the performance of solar cell devices as it together with the charge carrier lifetime defines the diffusion length of the charge carriers and hence sets a limit to the device active layer thickness. For lead halide perovskite (HaP) solar cells, long charge carrier diffusion lengths up to micrometer scale have been reported which is primarily due to the long charge carrier lifetime. However, the charge carrier mobility is found to be smaller compared to the theoretically predicted values. In order to investigate the fundamental charge carrier transport properties in HaP materials we used the contact-less technique of transient microwave conductivity (TRMC). We analysed different HaPs including methylammonium lead iodide ($MAPbI_3$), lead bromide ($MAPbBr_3$) and mixed cation and halide perovskite by TRMC at room temperature and find the highest charge carrier mobility for $MAPbI_3$. Finally, TRMC mobilities in $MAPbI_3$ tested in a wide temperature range show a clear negative temperature coefficient in the tetragonal phase as well as a mobility drop at the phase transition.

CPP 2.11 Mon 12:30 H18

Anisotropic charge carrier diffusion in methylammonium lead iodide — Ilka M. Hermes[1], Markus Mezger[1,2], David S. Ginger[3], Rüdiger Berger[1], Kaloian Koynov[1], and •Stefan A.L. Weber[1,2] — [1]MPI for Polymer Research, Mainz, Germany — [2]Institute of Physics, JGU Mainz, Germany — [3]University of Wahsington, Seattle, USA

In this combined piezoresponse force microscopy (PFM) and local time-resolved photoluminescence (PL) study, we correlate the charge carrier dynamics on large ($>10\mu$m) isolated methylammonium lead iodide grains to the arrangement of ferroelastic twin domains[1]. Using PL-microscopy, we measured the carrier diffusion parallel and perpendicular to the twin domain stripes. The diffusion parallel to the domains was significantly faster than perpendicular to the domains, resulting in a distinct anisotropy in the carrier dynamics. Our results demonstrate that controlling the strain during crystal growth could offer a way to enhance carrier extraction in perovskite solar cells. [1] J. Phys. Chem. C, 2016, 120, 5724.

CPP 3: Molecular Electronics and Excited State Properties

Time: Monday 9:30–13:00 Location: H13

Invited Talk CPP 3.1 Mon 9:30 H13

Tailoring the Excited State Energy Landscape in Supramolecular Nanostructures — •Richard Hildner — Soft Matter Spectroscopy, University of Bayreuth, Bayreuth, Germany — Zernike Institute for Advanced Materials, University of Groningen, Groningen, Netherlands

Application of organic macromolecules in molecular electronics and nanophotonics requires their well-defined assembly into nano- and mesoscale structures to allow for efficient energy and/or charge transport. Here we demonstrate robust self-assembly of so-called carbonyl-bridged triarylamines (CBT) into micrometre-long objects driven by specific supramolecular motifs. Depending on the solvent we are able to prepare isolated supramolecular nanofibres, in which the CBT molecules are cofacially stacked (H-aggregate), or to prepare well-defined bundles of such nanofibres. Combining optical spectroscopy with electron microscopy and numerical modelling, we find that isolated nanofibres possess a high degree of structural order. In turn, this results in a high degree of electronic order in the electronically excited states. In contrast, in nanofibre bundles the structural and electronic order is significantly less pronounced. We show that this difference in order has substantial impact on the transport of excitation energy: While isolated nanofibres exhibit long-range energy transport of several micrometres, in nanofibre bundles this is not the case. Hence, the solvent allows to tune the excited state energy landscape of nanofibres, which in turn allows to control the transport characteristics of excitation energy along nanofibres.

CPP 3.2 Mon 10:00 H13

Controlling H- and J-type electronic coupling in single deterministic conjugated polymer aggregates — •Theresa Eder[1], Christoph Allolio[2], Dominik Horinek[2], Sigurd Höger[3], Jan Vogelsang[1], and John M. Lupton[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]Institut für Physikalische und Theoretische Chemie, Universität Regensburg, Germany — [3]Kekulé-Institut für organische Chemie und Biochemie, Universität Bonn, Germany

The electronic coupling in conjugated polymers, which impacts the spectroscopic behavior tremendously, can be explained in the theoretical framework of H- and J-aggregation between neighboring chromophoric units. We investigate custom-synthesized model polymers and oligomers and show how the distance between chains impacts the coupling type [1]. Based on the work on single polymer aggregates, we intramolecularize aggregation by designing single dimers and trimers with a fixed spatial distance of the conjugated units. Here, we are also able to demonstrate, in combination with molecular dynamics and TDDFT calculations, that strong H-type coupling occurs in ordered oligomers at close spacings, whereas disorder and increased spacing quenches coupling [2]. Further, the examination of single-molecule spectra allows us to show how an increase in the dimer length with similar chromophore distance gives rise to increased J-type attributes such as spectral narrowing and reduced vibronic coupling.

[1] T. Eder et al., Nature Commun. 8, 1641 (2017)

[2] C. Allolio et al., J. Phys. Chem. B 122, 6431 (2018)

CPP 3.3 Mon 10:15 H13

Controlling Exciton Dynamics in Tetracene-Derivatives by Covalent Bounding of Two Chromophores — •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]ZAE Bayern, 97074 Würzburg

For an efficient operation of optoelectronic devices it is inevitable to control the photodynamics and, thus, the relevant loss channels like charge transfer formation or singlet fission (SF). In case of the latter, the excited singlet state decays into two triplet states of lower energy located on neighboring chromophores. Tetracene (Tc) is a model system to study this process and has motivated us to prove by rational design, here the covalent linking of two Tc chromophores, the effect of molecular packing on the optical properties and, in particular, on SF. By a comparative study on neat Tc and ditetracene (DTc) bulk crystals as well as anthracene crystals doped by the two entities at the single molecule level, different excitonic states can be identified together with the influence of the local environment and temperature. Quantities like spectral selective fluorescence lifetime, photoluminescence and absorption spectra as well as quantum efficiency are presented for each of the sample types studied, showing, as a key result, that SF is suppressed in DTc crystalline aggregates. Therefore, a model for the excitation energy landscape of DTc single crystals can be deduced and highlights the effect of the additional covalent bond on the photodynamics.

CPP 3.4 Mon 10:30 H13

Ultrafast excited state relaxation monitored by single molecule photon statistics — •Jakob Schedlbauer[1], Philipp Wilhelm[1], Maria-Elisabeth Federl[1], Florian Hinderer[2], Sigurd Höger[2], Lennart Grabenhorst[3], Phillip Tinnefeld[3], Jan Vogelsang[3], Sebastian Bange[1], and John M. Lupton[1] — [1]Universität Regensburg, Germany — [2]Universität Bonn, Germany — [3]LMU München, Germany

A new experimental approach is presented to monitor ultrafast excited state deactivation combining single molecule fluorescence spectroscopy (SMS) with a pump-probe-like excitation scheme. In the simplest way a single molecule can be described as a two level system and therefore can emit only one single photon after a given excitation pulse, a phenomenon referred to as photon antibunching. By introducing a second excitation pulse after a variable time lag the probability for reexciting the system and generating a second photon is a function of the excited state lifetime. A Hanbury-Brown-Twiss based detection setup enables us to measure the probability for the emission of multiple photons after a given excitation cycle.

This technique overcomes the limitation of conventional fluorescence based lifetime measurements such as time-correlated single-photon counting, which is constrained by finite detector instrument response function. We resolve dynamical single molecule processes like the intramolecular energy transfer in a acceptor-donor-acceptor system (13 ps) as well as ultrafast enhanced PL of Cy7 dyes coupled to a plasmonic antenna structure (20 ps).

CPP 3.5 Mon 10:45 H13

Simultaneous Singlet-Singlet and Triplet-Singlet Förster Transfer — •Anton Kirch, Max Gmelch, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, 01187 Dresden, Germany

We present our study of Förster resonant energy transfer (FRET) for the interesting case using a biluminescent donor material. FRET is used as spectroscopic ruler in various research fields and also determines many photonic and optoelectronic applications on the nanoscale. A biluminescent organic molecule is one that shows both fluorescence and phosphorescence at room temperature, where the latter is only observed under special conditions, which are currently widely explored in material research. The time dynamics of such a biluminophore is very special, spanning from nanoseconds-lifetime fluorescence to seconds-lifetime phosphorescence.

Here, we show that such a biluminescent donor can transfer its energy of both singlets and triplets to a fluorescent donor in the exact same framework of FRET. For both singlet and triplet energy transfer, we separately determine the nanoscale range (< 10 nm). The unified observation and description of singlet and triplet FRET from the very same molecular origin (same donor) has not been discussed in literature before. Importantly, our study validates Förster's theory on a single system over eight orders of magnitude in respective excited state lifetimes.

CPP 3.6 Mon 11:00 H13

Polarized absorbance and Davydov splitting in bulk and thin-film pentacene polymorphs — •Caterina Cocchi[1], Tobias Breuer[2], Gregor Witte[2], and Claudia Draxl[1] — [1]Physics Dept. and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — [2]Faculty of Physics, Philipps-Universität Marburg, Germany

Pentacene is one of the most studied organic materials but a number of issues related to it are still debated. One of them concerns the role of polymorphism and its effects on the lowest-energy excitations, appearing in the visible region and being subject to a sizable Davydov splitting. We address this problem in a combined theoretical and experimental work, where the electronic and optical properties of three pentacene phases (two bulk polymorphs and the thin-film phase) are investigated. Optical spectra computed from many-body perturbation theory are compared with the polarization-resolved absorbance. In this way, the two Davydov components of the first exciton are identified along with the optical fingerprints of each considered phase. All polymorphs exhibit common features at the absorption onset, while phase-dependent characteristics appear only above 2 eV. We discuss the character of the lowest-lying singlet and triplet excitons, highlighting the contributions from the electronic bands as well as the role of electron-hole interaction and local-field effects [1].

[1] C. Cocchi T. Breuer, G. Witte, and C. Draxl Phys. Chem. Chem. Phys. DOI: 10.1039/C8CP06384B (2018).

15 min. break

CPP 3.7 Mon 11:30 H13

Temperature Dependent Photoluminescence Studies on Zinc Phthalocyanine Single Crystals — •Larissa Lazarov[1], Sebastian Hammer[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

Zinc-phthalocyanine (ZnPc) has been one of the most studied materials in organic solar cells, due to its high photostability, electronic tunability and superior opto-electronic properties compared with other metal-phthalocyanines [1]. Remarkably, the microscopic photophysical processes in ordered ZnPc aggregates have not been studied in great detail so far. For this purpose, we grew ZnPc single crystals via gradient sublimation and confirmed their crystallographic β-phase by X-ray diffraction. Temperature dependent photoluminescence (PL) studies have been performed from 4 to 330 K. Below 100 K the radiative 0-0 vibronic transition consists of two narrow lines with a FWHM of about 20 meV, respectively. The emission intensity in this temperature range indicates superradiance accompanied by exciton delocalization over several molecules according to Spano's method [2]. Above 100 K, thermally activated aggregate emission appears to be the dominant process in PL enhancement by up to one order of magnitude at 330 K. We discuss the superradiant behavior in respect to its dependence on polarization and excitation power and shed light on the microscopic processes leading to the emission behavior at elevated temperatures.

[1] Brendel et al., *Adv. Funct. Mater.*, **25**, 2015

[2] Spano, F.C., Yamagata, H., *JPCB* **115**, 5133-5143, 2011

CPP 3.8 Mon 11:45 H13

Programmable transparent organic luminescent tags — •Max Gmelch, Heidi Thomas, Felix Fries, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, 01187 Dresden, Germany

A novel approach for organic luminescent labeling is shown, providing unmatched image resolution (>700 dpi) combined with fast and multiple (>40 cycles) printing onto and erasing from various substrates in any shape or size. These ultrathin, fully transparent and flexible organic tags contain highly available materials only and are easy to process. The material system consists of an organic biluminescent emitter, embedded into a PMMA host matrix and covered by an oxygen barrier layer. It shows room temperature phosphorescence (RTP), which in general is quenched by molecular oxygen. However, by illuminating with ultraviolet light, this molecular oxygen locally vanishes at the irradiated spots, enabling RTP at defined spots. Further, by illuminating with infrared light, the system can be refilled with oxygen leading to quenching of the RTP again. Therefore, any luminescent pattern can be written into and erased from the tag without contact or the use of any ink. Using light only, this new technology offers the possibility of invisible on-demand information readout.

CPP 3.9 Mon 12:00 H13

Absence of Charge Transfer States at Crystalline Perfluoropentacene/Pentacene Interfaces — •Sebastian Hammer[1], Clemens Zeiser[2], Katharina Broch[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Institute for Applied Physics, University of Tübingen, 72076 Tübingen — [3]ZAE Bayern, 97074 Würzburg

The formation of charge transfer (CT) states plays an important role in charge seperation and impacts the efficiency of organic photodetectors and photovoltaics. Pentacene:Perfluoropentacene (P:PFP) has been largely studied in mixed films as a prototypical CT system by its suited donor/acceptor (D/A) energy levels [1][2]. However, the role of molecular orientation on charge transfer has not been elucidated, so far. For this purpose, we used heteroepitaxial growth of PFP on P (001) crystal interfaces to achieve long-range ordered D/A heterojunctions of edge-on molecular orientation as confirmed via X-ray diffraction. By means of temperature dependent cw fluorescence spectroscopy and *in-situ* differential reflectance spectroscopy we determined the optical characteristics of the PFP/P thin films and demonstrate the absence of CT state formation at the generic (001) edge-on crystalline interface. We discuss these findings with respect to possible implementation in organic solar cells where the suppression of strongly bound CT states at D/A heterointerfaces yields an increase in open circuit voltage, and thus in device performance.

[1] K. Broch et al., *Phys. Rev. B* **83**, 245307 (2011)

[2] T. Breuer, G. Witte, *J. Chem. Phys.* **21**, 138 (2013)

CPP 3.10 Mon 12:15 H13

Interplay between intra- and inter-molecular charge transfer in the optical excitations of J-aggregates — •Michele Guerrini[1,2,3], Caterina Cocchi[2], Arrigo Calzolari[3], Daniele Varsano[3], and Stefano Corni[3,4] — [1]Dept. FIM, Univ. of Modena and Reggio Emilia, Italy — [2]Dept. of Physics and IRIS Adlershof, Humboldt Universität zu-Berlin, Germany — [3]CNR Nano, Centro S3, Modena, Italy — [4]Dept. Chem. Scienc., Univ. of Padova, Italy

Molecular J-aggregates formed by push-pull chromophores have appealing optical properties which are dominated by collective and supramolecular effects, as recently demonstrated from first principles [1]. Here, we investigate the character of the optical excitations from many-body perturbation theory, focusing on the interplay between intra- and inter-molecular interactions. We find that the most intense excitation which dominates the spectral onset (the so-called J-band) exhibits a combination of intra-molecular charge transfer, coming from the push-pull character of the constituting dyes, and inter-molecular charge-transfer, due to the dense molecular packing which favors wave-function delocalization. Within the J-band we also reveal the presence of a pure inter-molecular charge-transfer excitation. Our results [2] shed light into the microscopic character of optical excitations in J-aggregates and offer new perspectives for understanding the nature of collective excitations in organic molecular solids.

[1] M. Guerrini; A. Calzolari; S. Corni ACS Omega 2018, 3 (9), 10481-10486. [2] M. Guerrini; C. Cocchi; A. Calzolari; D. Varsano; S. Corni submitted (2018).

CPP 3.11 Mon 12:30 H13

Differentiation between the optical signatures of aggregates and of isolated chains in doped P3HT solutions — •Ahmed E. Mansour[1], Dominique Lungwitz[1], Thorsten Schultz[1], Andreas Opitz[1], and Norbert Koch[1,2] — [1]Institut für Physik & IRIS Adlershof, Humboldt Universität zu Berlin, Germany — [2]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Germany

Molecular doping of Poly(3-hexylthiophene-2,5-diyl) (P3HT) results in the formation of polarons as the main charge carriers. Charged polymer segments can be identified by optical absorption spectroscopy.[1,2] Furthermore, molecular doping typically may lead to aggregation of P3HT and the dopant already in the solution, which alters the film morphology.[3,4] Herein, we compare the optical signatures of doped aggregates and doped single chains in solution. Their relative size is compared by filtering doped suspensions for different absolute concentrations and dopant ratios. We find that doped single chains exhibit absorption features at 1.5 eV and 0.6 eV. For doped aggregates, the peak at higher absorption energy is split into two absorption features at 1.3 eV and 1.65 eV. Further, we show that the size of dopant induced aggregation increases as a function of absolute concentration and dopant ratio. Doped P3HT suspensions are shown to comprise both doped species, with the aggregates exhibiting a larger dopant loading.

[1]Bredas, J. L. et al., Acc. Chem. Res. 1985, 18, 309. [2]Heimel, G., ACS Cent. Sci. 2016, 2, 309. [3]McFarland, F. M. et al., J. Phys. Chem. C 2017, 121, 4740. [4]Jacobs, I. E. et al, J. Mater. Chem. C 2016, 4 (16), 3454.

CPP 3.12 Mon 12:45 H13

What is the impact of the donor length on the electronic and optical properties of charge-transfer complexes? — •Ana M Valencia and Caterina Cocchi — Physics Department, Humboldt-Universität zu Berlin und IRIS Adlershof

The size ratio between donor and acceptor moieties in organic semiconductors is know to effectively influence the doping mechanism [1]. Here, we investigate a series of charge transfer complexes formed by oligothiophene molecules of increasing length doped by the acceptor F4TCNQ. Using hybrid DFT as a starting point, we assess the electronic and optical properties of these systems from many-body perturbation theory (GW and the Bethe-Salpeter equation). We find that the frontier orbitals (HOMO and LUMO) are hybridized in all complexes, while the distribution of deeper occupied and higher virtual states depend on the nT length. The first bright excitation is dominated by the HOMO-LUMO transition occurring approximately at the same energy in all systems. At increasing donor length, higher-energy peaks exhibit different character depending on the donor conjugation length [2]. We also consider how the relative concentration of donor and acceptor molecules impacts these properties. The rationale offered by our results contributes to clarify the excitation processes in organic donor/acceptor complexes. [1] H. Mendez, et al., Nat. Comm. 6, 8560 (2015). [2] A.M. Valencia and C. Cocchi submitted (2018).

CPP 4: Responsive and Adaptive Systems (joint session CPP/DY)

Time: Monday 9:30–12:15 Location: H8

CPP 4.1 Mon 9:30 H8

H2O / D2O swelling and exchange kinetics of a multi-stimuli responsive PNIPAM-based block copolymer thin film — •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, James-Franck-Str. 1, 85748 Garching — [2]Helmholtz-Zentrum Geesthacht at Heinz Maier-Leibnitz Zentrum, Lichtenbergstr. 1, 85747 Garching — [3]Universität Potsdam, Institut für Chemie, Karl-Liebknecht-Straße 24-25, 14476 Potsdam Golm

Stimuli-responsive polymers can react with a drastic change in properties towards even slight changes in their surrounding environment. Especially in thin film morphology, such films are well-suited for a manifold of applications such as nano-switches, artificial muscles in soft-robotics or sensors. In order to implement stimuli-responsive polymers in the aforementioned application fields, a fundamental understanding of the underlying kinetics is necessary. In our recent work, we followed the H2O and D2O swelling and the corresponding exchange kinetics in a multi-stimuli responsive block copolymer thin film with in-situ time of flight (TOF) neutron reflectometry (NR). TOF-NR enables high time resolution with which the mechanisms of water uptake and exchange can be followed. A theoretical model is applied to describe the swelling and exchange kinetics in order to obtain detailed insights about the underlying mechanisms of these dynamic processes.

CPP 4.2 Mon 9:45 H8

Morphology of Thermoresponsive Molecular Brushes with Copolymer Side Arms in Aqueous Solution — •Jia-Jhen Kang[1], Junpeng Zhao[2], Henrich Frielinghaus[3], Lester Barnsley[3], Fabian Kohler[1], Hendrik Dietz[1], Stergios Pispas[2], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]National Hellenic Research Foundation, Theoretical and Physical Chemistry Institute, Athens, Greece — [3]FZ Jülich, JCNS at MLZ, Garching, Germany

Poly (ethylene oxide) (PEO) and poly (propylene oxide) (PPO) are known to be thermoresponsive polymers both exhibiting lower critical solution temperature (LCST) behavior, with the cloud points >100 °C and 8 °C, respectively. In the present work, we aim to investigate the LCST behavior of their densely-grafted analogues, namely molecular brushes, which are polymers composed of a polymeric backbone and side arms attached to virtually every monomer of the backbone. Molecular brushes with PEO-ran-PPO and PEO-block-PPO copolymer side arms were studied in aqueous solution using dynamic light scattering (DLS) and small angle neutron scattering (SANS). They display mixed LCST behavior based on the two components, indicating new properties induced by the densely-grafted architecture.

CPP 4.3 Mon 10:00 H8

Formation and growth of mesoglobules in aqueous poly(N-isopropylacrylamide) solutions at low and high pressures revealed with fast pressure jumps — •Bart-Jan Niebuur[1], Leonardo Chiappisi[2], Florian Jung[1], Xiaohan Zhang[1], Alfons Schulte[3], and Christine M. Papadakis[1] — [1]TU München, Physik Department, Physik weicher Materie, Garching, Germany — [2]Institut Laue-Langevin, Large Scale Structures Group, Grenoble, France — [3]University of Central Florida, Department of Physics and College of Optics and Photonics, Orlando, U.S.A.

Understanding the kinetics of phase separation is of importance for numerous systems. The thermoresponsive polymer poly(N-isopropylacrylamide) (PNIPAM) presents a model system to investigate the kinetics of phase separation. In aqueous solutions at temperatures above the cloud point, PNIPAM forms stable mesoglobules with their size and hydration state depending strongly on pressure [1]. To elucidate the formation and early stage growth of the mesoglobules, we applied time-resolved small-angle neutron scattering after rapid pressure jumps inducing phase separation at low and high pressures. We find that mesoglobule formation includes the formation of small clusters, growth by diffusion-limited coalescence, and the formation of a dense shell, slowing down further coalescence [2]. The strong dehydration at low pressures results in much slower kinetics than at high pressures, where the chains stay more hydrated. [1] B.-J. Niebuur, C. M. Papadakis et al., *ACS Macro Lett.* 2017, **6**, 1180. [2] B.-J. Niebuur, C. M. Papadakis et al., *ACS Macro Lett.* 2018, **7**, 1155

CPP 4.4 Mon 10:15 H8

The structural and dynamic behavior of the thermoresponsive polymer Poly(N-isopropylmethacrylamide) — •Chia-Hsin Ko[1], Kora-Lee Claude[1], Dirk Schanzenbach[2], Bart-Jan Niebuur[1], Henrich Frielinghaus[3], Lester Barnsley[3], Vitaliy Pipich[3], Alfons Schulte[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, Germany — [3]FZ Jülich, JCNS at MLZ, Garching, Germany — [4]University of Central Florida, Department of Physics, Orlando, U.S.A — [5]Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm, Germany

Poly(N-isopropylmethacrylamide) (PNIPMAM) is a thermoresponsive polymer, exhibiting lower critical solution temperature (LCST) behavior in aqueous solution. Compared to the well-investigated poly(N-isopropylacrylamide) (PNIPAM), which has similar chemical structure, PNIPMAM has a higher transition temperature (43 °C instead of 32 °C). This may be due to the presence of the additional methyl groups on the vinyl backbone, which cause steric hindrance and weaken the intramolecular interactions. We investigate the temperature- and concentration-dependent phase behavior of PNIPMAM in D_2O using turbidimetry, dynamic light scattering (DLS), small-angle neutron scattering (SANS) and Raman spectroscopy. The main difference from PNIPAM are inhomogeneities in the one-phase state due to physical crosslinks caused by the methyl groups.

CPP 4.5 Mon 10:30 H8

All-in-One 'Schizophrenic' Self-assembly of Orthogonally Tuned Thermo-responsive Diblock Copolymers — Natalya S. Vishnevetskaya[1], Viet Hildebrand[2], 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

Smart, fully orthogonal switching was realized in a diblock copolymer system with variable trigger-induced aqueous self-assembly [1]. The polymers are composed of non-ionic and zwitterionic blocks featuring lower and upper critical solution temperatures (LCST, UCST). Due to the salt-sensitivity of the zwitterionic block, the UCST can be varied by addition of salt. Superimposed orthogonal switching by electrolytes results in 'schizophrenic' micellization, in which the roles of the core and the shell block are interchanged. The following switching scenarios are observed by turbidimetry and SANS: i) via a molecularly dissolved state at low NaBr concentrations, or (ii) via an insoluble state at high NaBr concentrations. The versatile and tunable self-assembly of such diblock copolymers offers manifold opportunities, e.g. for smart emulsifiers.

1. N. S. Vishnevetskaya et al., Macromolecules 51, 2604 (2018)

CPP 4.6 Mon 10:45 H8

PNIPAM microgel-stabilized aqueous foams and foam films — •Matthias Kühnhammer and Regine von Klitzing — Technical University of Darmstadt, Soft Matter at Interfaces, Darmstadt, Germany

Cross-linked, short-chained poly-N-isopropylacrylamide (NIPAM) polymers have been in the focus of numerous studies in the past years and are still being discussed very actively in the context of multiple possible applications, because of their ability to respond to external stimuli like temperature. 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.

In this contribution the interfacial activity of PNIPAM microgels is exploited to stabilize aqueous foams. These foams are very stable at temperatures below the volume phase transition temperature (VPTT) of NIPAM and can be destabilized by increasing the temperature above the VPTT. In addition, the relation between the properties of individual microgels (e.g. size, elasticity, particle concentration) and the properties of foams prepared with them is studied. The properties of foam films are studied with a thin film pressure balance and are related to features of macroscopic foams investigated in drainage experiments and with neutron scattering.

CPP 4.7 Mon 11:00 H8

Reversible surface structuring of photosensitive polymer films: In-situ atomic force microscopy and diffraction efficiency measurements — •Joachim Jelken, Burkhard Stiller, Carsten Henkel, and Svetlana Santer — Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany

Here we report on light induced reversible structuring of azobenzene containing polymer films under dynamic changing of local distribution of electrical field vector in interference pattern used for the polymer irradiation. This is achieved utilizing a homemade setup which consists of three parts: a two beam interference setup for topography structuring, an atomic force microscope (AFM) for in-situ recording (during irradiation) of surface morphology[1,2], and a diffraction efficiency (DE) setup which enables to obtain information about the birefringence grating at the same time. Introducing a phase delay between the two interfering beams results in a shift of the whole interference pattern along the sample plane. Depending on the shifting speed the topography grating follows the redistribution of electrical field vector. In this way one can reversible structure and flatten surface topography in controlled manner. Using the measured kinetics of topography and birefringence gratings we aim to further understand the process of surface relief grating formation in azobenzene containing polymer films [3]. [1]S. N. Yadavalli, M. Saphiannikova and S. Santer, Appl. Phys. Lett., 2014, 105, 051601 [2]S. N. Yadavalli and S. Santer, J. of Appl. Phys., 2013, 113, 224304-12 [3]V. Toshchevikov, J. Ilnytskyi and M. Saphiannikova, J. Phys. Chem. Lett. 2017, 8, 1094

15 min. break

CPP 4.8 Mon 11:30 H8

Modelling of light-induced deformations in side-chain azopolymers — •Bharti Yadav, Jan Domurath, and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden e. V., Hohe Str. 6, 01069 Dresden

Photopolymers deform in the presence of light, even below the glass transition temperature, because the stress produced by the light is greater than the yield stress [1]. The deformations in the photopolymers are directional i.e. they depend on the polarization of light [2]. For linearly polarized light the deformation is in the direction of the polarization and for circularly polarized light in the plane perpendicular to the propagation vector. These directional deformations are caused by the light-induced orientation potential, which acts on each chromophore attached to the main chain. From the orientation potential one can calculate the light-induced stress in the sample. We model these photopolymers as visco-plastic materials by implementing the light-induced stress using ANSY, a finite element modelling software. We calculate the strain and elongation as a function of time for both linearly and circularly polarized light.

[1] Toshchevikov, V. et al. J. Phys. Chem. Lett. 8 (2017) p.1094-1098

[2] Kang., H. S. et al. Adv. Funct. Mater. 24 (2014) p.7273-7283

CPP 4.9 Mon 11:45 H8

Columnar clusters of three-arm azobenzene stars - MD simulations of a light-induced phase transition — •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, Germany

In this study we investigate star-shaped molecules consisting of a central benzenetricarboxamide (BTA) core and three symmetrically attached azobenzene groups. In aqueous solution these molecules exhibit a distinctive photoresponsive self-assembly behavior. In the absence of light or exposed to blue visible light they form long fibrous structures. When irradiated with UV light the columns disassemble but can be restored after resuming exposure to the initial conditions [1]. This phase transition is a result of the trans-cis photoisomerization of the centrally anchored azobenzene arms. We demonstrate, using DFT and MD simulations, that the solvophilicity of azo stars increases with the number of azo groups present in the cis state [2]. Further on using MD simulations, the stability of the columnar clusters in water is tested, while again varying the amount of trans and cis arms per molecule. Our results indicate that clusters with a large fraction of cis-arms display higher disorder or may even break apart. Lastly, also the kinetics of cluster self-assembly from random initial distributions is studied.

We gratefully acknowledge support from the German Research Foundation (DFG), projects GU 1510/3-1 and SA 1657/13-1.

[1] Lee, S. et al. Langmuir 29 (19), 5869 (2013)

[2] Koch, M. et al. J. Phys. Chem. B 121, 8854 (2017)

CPP 4.10 Mon 12:00 H8

Dissipative systems with nonlocal delayed feedback — •Josua Grawitter, Reinier van Buel, Christian Schaaf, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

We present a linear model, which mimics the response of a spatially extended dissipative medium to a distant perturbation and investigate its dynamics under delayed feedback control [Grawitter *et al.*, New J. Phys. **20**, 113010 (2018)]. In our model the time it takes a perturbation to travel to the location of measurement is described by an inherent delay time. We investigate the resulting double-delay differential equation using linear stability analysis and numerical integration.

For nonzero delay, linear stability analysis reveals that sufficiently strong feedback destabilizes the system's trivial fixed point. When feedback is bounded by a smooth sigmoid function, the stability-instability transition follows a supercritical Hopf bifurcation and a stable limit cycle occurs. Its frequency and amplitude respond to parameter changes like the dominant eigenvalue of the linearized problem. In particular, they show similar discontinuities along specific lines. These results are largely independent of the chosen sigmoid function and match previous findings on the feedback-induced instability of vortex diffusion in a rotationally driven Newtonian fluid. Because our model captures the essential features of nonlocal delayed feedback in dissipative systems, we consider it a valuable reference case for studies of more complex and spatially extended systems such as photoresponsive fluid interfaces.

CPP 5: Membranes and vesicles I (joint session BP/CPP)

Time: Monday 9:30–12:30 Location: H10

CPP 5.1 Mon 9:30 H10

Soft Thermal Treatment Stabilizes Vacuum-deposited Phospholipid Layers for Sensor Applications — Sebastian Molina[1], Marcelo Cisternas[1], Maria J. Retamal[2], Nicolas Moraga[1], Hugo Zelada[1], •Jonas Fortmann[1,3], Tomas P. Corrales[4], Patrick Huber[5], 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]TU Clausthal, Germany — [4]Department of Physics, UTFSM, Valparaiso, Chile — [5]TUHH, Hamburg, Germany

Artificial membranes allow one to study of the behavior of biological membranes, which are the base of the cell membrane structure. The cell membrane is composed of different lipids and proteins that change their behavior when they are stimulated physically and/or chemically. Besides traditional methods we use a solvent free, dry method for phospholipid deposition in high vacuum onto residue-free silicon substrates. The cleanness of the substrate and the precise thickness of the DPPC layer on the substrate is controlled in-situ using Very High Resolution Ellipsometry. In this work we show the enhancement of phospholipid bilayer self-assembling and stability due to a soft thermal treatment. The behavior of the artificial membranes is studied in air and immersed in aqueous medium, which mimics the natural environment of the biological membrane. Acknowledgements: FONDECYT Nos. 3160803 (MJR), 1180939 (UGV) 1171047 (MSA) and 11160664 (TPC), CONICYT Fellowship (MC) and CONICYT-PIA ACT 1409.

CPP 5.2 Mon 9:45 H10

Prolonged Phospholipid Bilayer Stability due to Hydration on Porous Silicon: Pore Diameter and Porosity Optimization — 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 artificial membranes has become an important way to gain insight into the physical behavior of cell membranes. In this work, porous silicon substrates (pSi) were prepared with different pore diameters and porosities. The 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 in-situ 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 show that specific pore diameters and porosities of nanoporous substrates prolong phospholipid bilayer stability due to hydration with water stored in the pores. Acknowledgement: FONDECYT Nos. 3160803 (MJR), 1180939 (UGV), 1171047 (MSA) and 11160664 (TPC), CONICYT Fellowship (MC) and CONICYT-PIA ACT 1409.

CPP 5.3 Mon 10:00 H10

Mechanisms of Interactions between Lipid Membranes in the Presence of Biological Cosolutes — •Amanuel Wolde-Kidan[1], Quoc Dat Pham[2], Alexander Schlaich[3], Emma Sparr[2], and Roland Netz[4] — [1]Freie Universität, Berlin, Germany — [2]Lund University, Lund, Sweden — [3]Laboratoire Interdisciplinaire de Physique, Grenoble, France — [4]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Lipid membranes form the diffusional barrier of eukaryotic cells and determine processes when cells come into close contact, for example during cell fusion or vesicle formation. We analyze the effects of three cosolutes on membrane interactions, which are all abundantly found in biological systems, namely urea, TMAO and sodium chloride. The effect of the polar solutes urea and TMAO on protein stability has been studied extensively, but their influence on lipid bilayers has only recently started to be investigated. Using atomistic molecular dynamics simulations and theoretical modeling we analyze different mechanisms of lipid-solute and lipid-lipid interactions. By means of solution thermodynamics we model the effect of the cosolutes on the hydration repulsion between lipid bilayers. Results from our simulations compare well to experimental calorimetric measurements. We find that the osmotic pressure due to the added solute has the most important influence on the hydration repulsion. Furthermore, we find that the interaction mechanism of sodium chloride with lipid bilayers is dominated by the ion-membrane potentials of mean force. Other factors such as the dielectric response seem to be of less importance.

CPP 5.4 Mon 10:15 H10

Glycolipids as zippers between phospholipid membranes — •Victoria Latza[1], Bruno Demé[2], and Emanuel Schneck[1] — [1]Max-Planck Institut für Kolloid und Grenzflächenforschung, Potsdam, Germany — [2]Institut Laue-Langevin, Grenoble, France

Essential mechanisms in biological cells, such as molecular transport and cell division, involve the spatiotemporal reorganization of membranes in terms of membrane adhesion or vesicle release. These processes are largely determined by membrane-membrane interactions and thus highly sensitive to the membranes* surface chemistry. It is known that certain membrane-bound saccharide motifs, such as the LewisX trisaccharide, promote membrane adhesion. These cases, however, have been viewed as exceptions. Here, with the help of small-angle x-ray scattering, we investigate the interaction between membranes composed of ternary lipid mixtures of (i) uncharged phospholipids as matrix, (ii) negatively charged phospholipids to induce electrostatic repulsion, and (iii) glycolipids featuring various mono- and oligosaccharide headgroups. We find that a large fraction of saccharide types are able to induce membrane adhesion through the formation of weak inter-membrane bonds. These bonds are resistant to electrostatic repulsion at levels that lead to the complete unbinding of pure phospholipid membranes. Our results strongly indicate that glycolipid-induced membrane-binding is not an exceptional feature of few saccharide types but a highly abundant phenomenon of great relevance for membrane biophysics.

Invited Talk CPP 5.5 Mon 10:30 H10

Lessons learned from complex mimics of biological membranes — •Georg Pabst — University of Graz, Institute of Molecular Biosciences, NAWI Graz, 8010 Graz, Austria

Lipid-only mimics of biological membranes serve as valuable platforms for studying the functional role of membrane lipids under chemically and experimentally well-defined conditions. Of recent, we have focused on complex mimics of mammalian and bacterial plasma membranes with either lateral or transbilayer inhomogeneities. In particular, we have developed protocols for fabricating and analyzing asymmetric lipid vesicles, which are sufficiently stable and which are amenable for biophysical studies using diverse techniques. We have specialized on small-angle X-ray/neutron scattering combined with complimentary techniques to address leaflet specific structure and transbilayer coupling mechanisms. Complementary, we are currently developing tools for reliable estimates for intrinsic lipid curvatures, which are known to play a pivotal role in coupling to protein function. I will present recent research highlights resulting from these efforts and discuss some applications to membrane-active drugs, such as antimicrobial peptides, or the partitioning of transmembrane proteins function.

30 minutes break.

CPP 5.6 Mon 11:30 H10

The interaction of viral fusion peptides with model lipid membranes at high hydrostatic pressure — Göran Surmeier[1], Michael Paulus[1], Susanne Dogan[1], Yury Forov[1], Mirko Elbers[1], Simon Egger[2] und •Julia Nase[1] — [1]Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund — [2]Physikalische Chemie, TU Dortmund, 44221 Dortmund

When a virus enters a host cell, the insertion of viral fusion peptides (FPs) into the target membrane catalyzes the membrane fusion reaction. We investigated the interaction of different FPs with model membranes in X-ray reflectivity measurements at the interface between monoolein/water mixtures and a silicon substrate. In addition, the bulk and interfacial structures were investigated with small angle X-ray scattering in transmission and in grazing incidence. Monoolein/water mixtures have a very rich pressure-dependent phase diagram. Notably, the inverse bicontinuous cubic phases exhibit structural analogies to the hemifusion intermediates. We found that pressurization triggers formation of ordered lamellar monoolein multilayers close to the interface even in a pressure range where the bulk material is in the cubic phase. Previous studies demonstrated the effect of FPs on the pressure-dependent phase boundaries [1]. We resolved the vertical membrane structure of some multilayers and monitored the penetration of FPs into the membrane. Experiments were performed in a custom-made high hydrostatic pressure cell [2] at beamlines ID31 of the ESRF and BL9 of DELTA. [1] A. Levin et al, J Phys Chem B 121 (2017) [2] F.J. Wirkert et al, J. Synchr. Radiat. 21 (2014)

CPP 5.7 Mon 11:45 H10

Lipid membrane fusion in proteoliposomes and multilamellar stacks studied by X-ray scattering — •Kilian Frank[1], Karlo Komorowski[1], Veronica Chappa[2], Max Scheu[1], Marcus Müller[2], and Tim Salditt[1] — [1]Georg-August-Universität, Institute for X-ray Physics, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Georg-August-Universität, Institute for Theoretical Physics, Friedrich-Hund-Platz 1, 37077 Göttingen

Intermediate structures of membrane fusion, e.g. during release of neurotransmitter at the synapse, are difficult to resolve at the molecular level, especially in the close-to-physiological regime with SNARE fusion proteins. To provide structural information, we combine two X-ray scattering approaches: First, SAXS on proteoliposomes (PL) with reconstituted SNAREs serves to identify changes in PL size and radial density profile upon fusion in a hydrated environment. We present a simulation framework based on 3D-FFT to estimate how well size and shape changes (homogeneous swelling of an ensemble, thermal fluctuations, and strong equilibrium defomations) are detected in PL-SAXS. Second, GISAXS on solid-supported multilamellar membrane stacks at controlled humidity and salt concentration allows to characterize the energy of fusion stalk formation, prior to crystallization to a stalk phase with rhombohedral symmetry. Here we find that CaCl2, in contrast to other salts, facilitates stalk phase formation, also cooperatively in fusiogenic lipid mixtures. By combining both methods, we lay the foundation for a quantitative X-ray analysis of the membrane fusion process with natural proteins or artificial peptides.

CPP 5.8 Mon 12:00 H10

Structural changes in biomimetic myelin membranes induced by Myelin Basic Protein — •Benjamin Krugmann[1,2], Andreas Stadler[1], Aurel Radulescu[2], Alexandros Koutsioumpas[2], and Stephan Förster[1,2] — [1]Forschungszentrum Jülich JCNS-1, 52428 Jülich, Germany — [2]Forschungszentrum Jülich JCNS-MLZ, 85748 Garching, Germany

The myelin sheath plays an important role in nerve signal conduction. It acts as an insulating layer which enables fast signal transport by reducing conduction losses. In demyelinating diseases like multiple sclerosis, this membrane is damaged, which leads to severe problems in nerve conduction. In literature different values for the lipid composition of healthy and modified membranes have been found. Based on these results, we investigate the membrane structure for the respective compositions. As next step we add Myelin Basic Protein (MBP) to the membrane and investigate the induced structural change. Small angle neutron scattering (SANS) and cryo-transmission electron microscopy data show the structure of vesicles with healthy and modified membrane composition and the strong structure change induced by MBP. Neutron Reflectometry (NR) data indicates that MBP interacts differently with healthy and modified myelin membranes.

CPP 5.9 Mon 12:15 H10

Influenza A matrix protein (M1) multimerization is the main driving force for membrane bending and tubulation. — •Ismail Dahmani — Cell Membrane Biophysics Group / Universität Potsdam Karl-Liebknecht-Str. 24-25, Haus 25, B/1.04 14476 Potsdam-Golm Deutschland

The matrix protein of the Influenza A virus (M1) forms a shell underlying the viral lipid envelope and controls the geometry of the virus capsid. In infected cells, M1 orchestrates the process of new virion formation by binding to the inner leaflet of the plasma membrane (PM), which finally results in bending of the lipid bilayer and virus release . The exact role of M1 polymerization in inducing membrane deformation and budding is not clear. Here, to model virus egress through the PM, we analyzed M1 binding to giant unilamellar vesicles (GUVs). Our results show that M1 and a construct consisting of its Nterminal domain (NM1) bind to negatively charged lipids causing unidirectional deformation by imposing an inward curvature and membrane tabulation . Detergent-mediated solubilization of the lipid bilayer after M1 binding leaves the three-dimensional organization of the protein intact, indicating that M1 forms a very stable network adjacent and independent from the lipid membrane. Our data also indicate that the C-terminal domain of M1 is not needed for the establishment of protein-protein interactions and membrane deformation. Finally in acidic conditions (pH=5) M1 irreversibly loses its ability to multimerize and induce curvature, thus confirming that M1 multimerization is the molecular mechanism responsible for membrane deformation.

CPP 6: Active Matter A (joint session DY/CPP)

Time: Monday 9:30–12:45 Location: H20

Invited Talk CPP 6.1 Mon 9:30 H20

Collective behavior and self-organisation of active granular particles — •Thorsten Pöschel, Michael Engel, Christian Scholz, and Harol Torres — Friedrich-Alexander-Universität Erlangen-Nürnberg

Biological organisms and artificial active particles self-organize into swarms and patterns. Open questions concern the design of emergent phenomena by choosing appropriate forms of activity and particle interactions. A particularly simple and versatile system are 3D-printed robots on a vibrating table that can perform self-propelled and self-spinning motion. Here we study a mixture of minimalistic clockwise and counter-clockwise rotating robots, called rotors. Our experiments show that rotors move collectively and exhibit super-diffusive interfacial motion and phase separate via spinodal decomposition. On long time scales, confinement favors symmetric demixing patterns. By mapping rotor motion on a Langevin equation with a constant driving torque and by comparison with computer simulations, we demonstrate that our macroscopic system is a form of active soft matter.

C. Scholz, T. Pöschel, Phys. Rev. Lett. 118, 198003 (2017)

C. Scholz, M. Engel, T. Pöschel, Nature Comm. 9, 931 (2018)

C. Scholz, S. D'Silva, T. Pöschel, New J. Phys. 18, 123001 (2016)

C. Scholz, T. Pöschel, Revista Cubana de Física 34, 69 (2017)

CPP 6.2 Mon 10:00 H20

Approximating microswimmer dynamics by active Brownian motion: Energetics and efficiency — •Jannik Ehrich and Marcel Kahlen — Institut für Physik, Carl von Ossietzky Universität, 26111 Oldenburg, Germany

We consider the dynamics of a microswimmer and show that they can be approximated by active Brownian motion. The swimmer is modeled by coupled overdamped Langevin equations with periodic driving. We compare the energy dissipation of the real swimmer to that of the active Brownian motion model finding that the latter can massively underestimate the complete dissipation. This discrepancy is related to the inability to infer the full dissipation from partial observation of the complete system. We introduce an efficiency that measures how much of the dissipated energy is spent on forward propulsion.

[1] J. Ehrich and M. Kahlen, arXiv:1809.07235 (2018)

CPP 6.3 Mon 10:15 H20

Magnetocapillary Microswimmers — •Maxime Hubert[1,2], Galien Grosjean[2], and Nicolas Vandewalle[2] — [1]PULS group, Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]GRASP Lab, CESAM UR, University of Liège, Liège, Belgium

The study of artificial microswimmers is of major interest in many area of physics, from the understanding of microorganisms swimming strategies to applications in microfluidic and micromanipulation. While there exists numerous theoretical studies on microswimmers, experimental realizations are technologically challenging. We focus in this presentation on a simple system made of three soft ferromagnetic particles trapped at air-water interfaces and self-assembling in triangles. Complex behaviors can arise under a time-dependent magnetic field. In particular, those assemblies can undergo deformations in non-time-reversible sequences, a necessary condition for low Reynolds number locomotion. Because of their controllability, such structures can be used for capture, transport and release of a microcargo, or the mixing of fluids at low Reynolds number. During this talk, the key mechanism for the collective motion of the beads is described from a numerical point of view and a model for their dynamics is discussed, opening the way for optimal control and efficiency of experimental magnetocapillary microswimmers.

CPP 6.4 Mon 10:30 H20

Self-assembly of dipolar active Brownian particles in two dimensions — •Guo-Jun Liao and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

We computationally study the self-assembly behavior of self-propelled Brownian particles with additional dipole-dipole interactions, stemming from a point dipole in the particle center. The propulsion direction of each particle is parallel to its dipole moment. At low densities and small dipolar coupling, the system undergoes a transition from a homogeneous state to a state with finite-sized (and orientationally disordered) clusters, when the particle motility is increased. Such cluster formation could be regarded as the asymptotic behavior of conventional active Brownian particles [1]. For strongly coupled dipolar colloids and zero motility, the model exhibits gel-like structures. On increasing particle motility, we observe a transition into a state with orientationally-ordered, finite-sized clusters. We analyze this state via the cluster size distribution and the net orientation. We also propose a mechanism to describe the emergence of such clusters.

Reference:

[1] G.-J. Liao and S. H. L. Klapp, Soft Matter 14, 7873 (2018)

CPP 6.5 Mon 10:45 H20

Experimental optimization of escape strategies in active systems. — •Hugo Wendehenne, François Lavergne, and Clemens Bechinger — Department of Physics, University of Konstanz, 78464 Konstanz, Germany

Groups formed by living organisms frequently react to external perturbations which can be repulsive (incoming predator) or attractive (presence of food). These responses are a combination of individuals reacting directly to the perturbation and collective mechanisms within the group. However, it is unclear whether collective interactions are a real benefit for an individual to escape from a repulsive perturbation. Here, we show that a change of the individuals' motilities and polarities in response to their visual perception of a perturbation leads to an effective escaping motion. Experimentally, this is demonstrated using active particles whose propulsion velocities and orientations are individually light-controlled by an external feedback-loop. We show that for a single active particle reacting to the perturbation within a restricted field of view, there is an increase of its rotational diffusion. The escape dynamics is characterized by ballistic transport, which is maximized for an optimal width of the particle's field of view. Interestingly, for a multi-particle system where individuals interact with their peers using a cohesion-based mechanism, we show that the escaping motion becomes more efficient. We expect this escaping mechanism to be relevant for cases where the perturbation is mobile, such as prey-predator interactions.

CPP 6.6 Mon 11:00 H20

Dynamics and configurations of active polymers — •Paolo Malgaretti — Max Planck Institute for Intelligent Systems, Stuttgart, Germany

We study the dynamics and conformation of polymers composed by active monomers. By means of Brownian dynamics simulations we show that, when the direction of the self-propulsion of each monomer is aligned with the backbone, the polymer undergoes a coil-to-globulelike transition, highlighted by a marked change of the scaling exponent of the gyration radius. Concurrently, the diffusion coefficient of the center of mass of the polymer becomes essentially independent of the polymer size for sufficiently long polymers or large magnitudes of the self-propulsion. These effects are reduced when the self-propulsion of the monomers is not bound to be tangent to the backbone of the polymer. Our results, rationalized by a minimal stochastic model, open new routes for activity-controlled polymers and, possibly, for a new generation of polymer-based drug carriers[1].

[1] V. Bianco, E.Locatelli, P. Malgaretti PRL 121, 217802 (2018)

15 min. break

CPP 6.7 Mon 11:30 H20

Collapse Dynamics of Polymers with Vicsek-like Activity — •Subhajit Paul[1], Suman Majumder[1], Subir K Das[2], and Wolfhard Janke[1] — [1]Institute for Theoretical Physics, University of Leipzig, Leipzig, Germany. — [2]Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur P.O., Bangalore, India

Many biologically active systems can effectively be understood within the framework of active matter models in statistical physics. In this regard, even modeling a single component Lennard-Jones-type fluid with Vicsek-like activity shows both rich phase and dynamical behavior. Motivated by this we construct a flexible bead-spring polymer model with Vicsek-like activity of the monomer beads. We pay particular emphasis on exploring the pathways of its collapse, following a quench from a high-temperature random coil state into a low-temperature phase where the equilibrium phase is a compact globule in the passive limit of the model. In the active case, however, our results from molecular dynamics simulations reveal that depending upon the strength of activity there is a rich phase behavior of the model that ranges from compact globule to dumbbells. On the nonequilibrium dynamics front, we compare our results with the passive polymer case, from the perspective of various scaling laws related to the collapse time, cluster coarsening, etc.

CPP 6.8 Mon 11:45 H20

Collective guiding of self-acoustophoretic particles in complex environments*

— Tobias Nitschke and •Raphael Wittkowski — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

Using self-propelled microparticles for medical applications like targeted drug delivery has been a dream for many decades. With the recent discovery of self-acoustophoretic particles, which move when they are exposed to ultrasound, a new type of particles with a biocompatible propulsion mechanism has become available. It turned out that these particles can be made from biocompatible materials and be equipped with mechanisms for the encapsulation and release of drugs. However, the hitherto insufficient capabilities for controlling the collective motion of the particles remained as a big obstacle preventing far-reaching medical applications.

In this talk, we present a method that allows to guide a large number of self-acoustophoretic particles collectively to a prescribed target region. The method is based on combining a moving focused ultrasound beam with a synchronized time-dependent magnetic field. Our method is harmless to patients and works even in complex environments like a patient's vasculature, when the particles are distributed throughout the body, and without information about the positions or orientations of the particles. Furthermore, we present a particle design that is particularly advantageous for applications.

**Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1*

CPP 6.9 Mon 12:00 H20

Emergent biomechanics in growing bacterial colonies

— •Anupam Sengupta — Physics of Living Matter Group, Physics and Materials Science Research Unit, University of Luxembourg

Bacterial colonies, known to mediate key ecological and industrial processes, constitute a class of active matter within which geometry, order, and topology emerge spontaneously over the lifespan of a colony. Although numerous studies have been carried out on growing colonies, so far we have lacked a comprehensive biomechanical framework that could capture the cell-to-colony dynamics and the consequences thereof. In this talk I will present recent results [1] obtained by combining micro-scale experiments, molecular dynamics simulations, and continuous modeling, that capture the continuous evolution of the geometry, order and topology in a growing colony of non-motile strain of E.coli bacteria. We reveal how steric forces between neighboring cells (favoring cell alignment), compete with the extensile stresses due to the cell growth (reducing the local order), leading to emergent biomechanics within the growing colony: spontaneous hydrodynamic flows, anisotropy of internal stresses, and emergent motility due to non-motile cells. The results indicate at activity-driven cell-cell communications preceding biofilm formation, and can be extended beyond bacterial communities, for instance, to study mammalian cells, many of which exist as non-motile elongated phenotypes.

[1] Geometry and Mechanics of Microdomains in Growing Bacterial Colonies: Z. You, D. Pearce, A. Sengupta*, and L. Giomi*, Phys. Rev. X 8, 031065, 2018.

CPP 6.10 Mon 12:15 H20

Phase transitions in huddling emperor penguins

— •Alexander Winterl[1], Sebastian Richter[1,2], Richard Gerum[1], Ben Fabry[1], and Daniel Paranhos Zitterbart[1,2] — [1]Biophysics Group, Friedrich-Alexander University, Erlangen, Germany — [2]Applied Ocean Physics and Engineering, Woods Hole Oceanographic Institution, Woods Hole, MA 02543, United States of America

Emperor penguins (*Aptenodytes forsteri*) breed under the harsh conditions of the Antarctic winter. To save energy and survive for 120 days of fasting, they from tight huddles. Using time-lapse images of an emperor penguin colony in Terre Adelie, we study huddle formation in response to environmental conditions (temperature, humidity, solar radiation, and wind speed). Huddle formation can be described as a phase transition from a freely moving state to a solid-like state where individual movements stall. We find a larger huddling probability with decreasing temperature and solar radiation and with increasing wind speed and humidity. These environmental factors can be lumped to an apparent temperature that would result in the same huddling probability in the absence of wind, humidity, and solar radiation, with weights of 1°C/°C for temperature, 2.9°C/(m/s) for wind, 0.5°C/% for rel. humidity, and $0.3°C/(W/m^2)$ for solar radiation. For the month of May, we find a critical temperature of −48.2°C for a 50% huddling probability. We expect this critical temperature to rise during fasting as the animals consume their insulating fat layer, and propose that the critical temperature can serve as an indicator for energy reserves and thus colony health.

CPP 6.11 Mon 12:30 H20

Delayed feedback control of active particles: a controlled journey towards the destination

— Seyed Mohsen Jebreiil Khadem and •Sabine H. L. Klapp — Institut für Theoretische Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin.

We explore theoretically the navigation of an active particle based on delayed feedback control. The delayed feedback enters in our expression for the particle orientation which, for an active particle, determines (up to noise) the direction of motion in the next time step. Here we estimate the orientation by comparing the delayed position of the particle with the actual one. This method does not require any real-time monitoring of the particle orientation and may thus be relevant also for controlling sub-micron sized particles, where the imaging process is not easily feasible. We apply the delayed feedback strategy to two experimentally relevant situations, namely, optical trapping and photon nudging. To investigate the performance of our strategy, we calculate the mean arrival time analytically (exploiting a small-delay approximation) and by simulations.

References:

[1] S. M. J. Khadem and Sabine H. L. Klapp arXiv:1811.06849v2 (2018).

CPP 7: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge I (joint session O/TT/CPP/DS)

First-principles electronic structure calculations have become an indispensable tool in many research areas where materials surfaces or interfaces play a central role. Corresponding calculations provide insight into catalytic mechanisms, interfacial ionic and charge transport in batteries or solar cells, materials degradation through corrosion or wear, and many other highly relevant application areas. Despite this prolific use, corresponding calculations face multiple issues. While the invited lectures will have a focus on this interface challenge, the symposium will also cover the general field of computational materials science and electronic-structure theory.

Organizers: Jens Nørskov (Technical University of Denmark), Karsten Reuter (Technical University Munich), and Matthias Scheffler (Fritz Haber Institute of the Max Planck Society, Berlin)

Time: Monday 10:30–13:00 Location: H9

Topical Talk CPP 7.1 Mon 10:30 H9

Scaling relations and beyond for kinetic Monte Carlo models in heterogeneous catalysis — •Mie Andersen — Theoretical Chemistry, Technische Universität München, Germany

Heterogeneous catalysis typically operates at the interface between a gas or liquid and a solid catalytic material. In my talk, I will discuss mean-field and kinetic Monte Carlo models for the operating catalyst. These often rely on input data calculated using either first principles or more approximate methods, e.g. scaling relations, which use only selected adsorption energies as descriptors for the catalyst function [1,2]. I will also discuss recent work [3] where we used compressed sensing methods to identify new low-cost and accurate descriptors that allow to predict adsorption energies for a wide range of adsorbates, multimetallic transition metal surfaces and facets. The descriptors are expressed as non-linear functions of intrinsic properties of the clean catalyst surface, e.g. coordination numbers and *d*-band moments. From a single DFT calculation of these properties, we predict adsorption energies at all potential surface sites, and thereby also the most stable geometry. Compared to previous approaches such as scaling relations, we find our approach to be both more general and more accurate for the prediction of adsorption energies on alloys with mixed-metal surfaces, already when based on training data including only pure metals.

[1] M. Andersen *et al.*, Ang. Chem. Int. Ed. **55**, 5210 (2016)
[2] M. Andersen *et al.*, J. Chem. Phys. **147**, 152705 (2017)
[3] M. Andersen *et al.*, submitted

CPP 7.2 Mon 11:00 H9

The Teacher and the Student: Exchange-Correlation Energy Densities from Quantum Chemistry and Machine-Learning — •Johannes T. Margraf, Christian Kunkel, and Karsten Reuter — Chair for Theoretical Chemistry, Technische Universität München, Germany

(Semi-)local density functional approximations (DFAs) are the workhorse electronic structure methods in condensed matter theory and surface science. Central to defining such DFAs is the exchange-correlation energy density ϵ_{xc}, a spatial function that yields the exchange-correlation energy E_{xc} upon integration.

Unlike E_{xc}, ϵ_{xc} is not uniquely defined. Indeed, there are infinitely many functions that integrate to the correct E_{xc} for a given electron density ρ. The challenge for constructing a useful DFA is to find a systematic connection between ρ and ϵ_{xc}. While several empirical and rigorous approaches to this problem are known, there has been little innovation with respect to the fundamental functional forms of DFAs in recent years.

Herein, we discuss two less explored routes to constructing DFAs. Specifically, a recipe for deriving ϵ_{xc} directly from many-body wavefunctions is compared to a machine learning (ML) approach that infers the optimal ϵ_{xc} for a given functional form. We find that local DFAs based on the many-body ϵ_{xc} are not transferrable between systems because the underlying energy densities are inherently non-local. In contrast, the ML ϵ_{xc} is by construction as local as possible. The extension of both approaches to non-local DFAs will be discussed.

CPP 7.3 Mon 11:15 H9

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

Electronic self-interaction is the most severe cause of inaccuracies in all semilocal density-functional approximations (DFAs), including the promising meta-GGA "strongly constrained and appropriately normed" (SCAN) functional [1]. This error can be alleviated via localized orbital scaling corrections [2] or via self-interaction corrections (SIC) based on Fermi-orbitals [3]. In this contribution, we follow the latter concept which involves solving a set of SIC constraints. Here, we present an all-electron implementation of the self-consistent SIC for semilocal DFAs, including SCAN. We first validate our implementation by inspecting certain properties (HOMO and dissociation energies) for a molecular test set, showing that SIC improves SCAN calculations. Furthermore, we compare the performance of SCAN-SIC and SCANα, i.e., SCAN with a fraction of exact exchange, in predicting the broken symmetry in pentacene – note that standard semilocal DFAs always favor symmetric solutions. Eventually, we discuss the extension of our SIC approach to periodic solids.

[1] J. Sun *et al.*, *Phys. Rev. Lett.* **115**, 036402 (2015).
[2] N. Q. Su *et al.*, *Proc. Natl. Acad. Sci.* **115**, 9678 (2018).
[3] Z. Yan *et al.*, *Phys. Rev. A* **95**, 052505 (2017).

CPP 7.4 Mon 11:30 H9

Progress in Fermi-Löwdin orbital self-interaction correction to DFT — •Torsten Hahn, Sebastian Schwalbe, and Jens Kortus — Institute for Theoretical Physics, Freiberg, Germany

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 selected applications. In addition we discuss strategies to improve the thermochemical and numerical performance of the FLO-SIC approach in combination with state-of-the-art exchange-correlation functionals.

[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] S. Schwalbe et al., J. Comp. Chem., vol. 39, 2463 (2018).

CPP 7.5 Mon 11:45 H9

Time evolution of the natural occupation numbers — •Carlos Benavides-Riveros and Miguel A. L. Marques — Martin-Luther Universität Halle Wittenberg

Reduced density matrix functional theory (RDMFT) is based on the Gilbert theorem, which asserts that the ground-state wave function can be written as a functional of the one-body reduced density matrix. Since RDMFT accounts for fractional natural occupation numbers, it captures quite well static (strong) electron correlation (unlike DFT, RDMFT correctly predicts the insulating behavior of Mott-type insulators). Yet the time-dependent extension of RDMFT suffers from various shortcomings. Chief among them, the current status of the theory does not allow the fermionic occupation numbers to evolve in time. It is known that this deficiency is connected to the failure of RDMFT to account for relative phases at the level of the two-body reduced density matrix. Based on recent results on fermionic exchange symmetry, we propose a new equation for the time evolution of the fermionic occupation numbers.

CPP 7.6 Mon 12:00 H9

Nonempricial hybrid functionals constructed through ad-

justable potential probes for band gap predictions of extended systems — •Thomas Bischoff, Igor Reshetnyak, and Alfredo Pasquarello — Chaire de Simulation a l'Echelle Atomique (CSEA), Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

We describe a nonempirical procedure for achieving accurate band gaps of extended systems through the insertion of suitably defined potential probes. By enforcing Koopmans' condition on the resulting localized electronic states, we determine the optimal fraction of Fock exchange to be used in the adopted hybrid functional. As potential probes, we consider native defects, the extrinsic hydrogen impurity, and various adjustable potentials that allow us to vary the energy level of the localized state in the band gap and its degree of localization. By monitoring the delocalized screening charge, we achieve a measure of the hybridization with the band states, which can be used to improve the band gap estimate. Application of this methodology to AlP, C and MgO yields band gaps differing by less than 0.2 eV from experiment.

CPP 7.7 Mon 12:15 H9

Quantum-mechanical relation between atomic dipole polarizability and van der Waals radius — •Dmitry Fedorov, Mainak Sadhukhan, Martin Stöhr, and Alexandre Tkatchenko — University of Luxembourg, Luxembourg, Luxembourg

The atomic dipole polarizability α and the van der Waals (vdW) radius $R_{\rm vdW}$ are two key quantities to describe the ubiquitous vdW forces important for the structure and dynamics of molecules and materials [1]. The commonly assumed relation between them, $R_{\rm vdW} \propto \alpha^{1/3}$, is based on a classical picture of hard-sphere atoms. Employing the quantum Drude oscillator model [2], we reveal [3] the quantum-mechanical relation $R_{\rm vdW} = const. \times \alpha^{1/7}$ which is markedly different from its classical counterpart. Based on the accessible accurate reference data for α and $R_{\rm vdW}$, we demonstrate that the obtained formula can be used as a unified definition of the vdW radius solely in terms of the atomic polarizability for all chemical elements. Moreover, for vdW-bonded heteronuclear dimers consisting of atoms A and B, the simple combination rule $\alpha = (\alpha_A + \alpha_B)/2$ provides a remarkably accurate way to calculate their equilibrium interatomic distance. These findings unveil a fundamental relationship between the geometric and electronic properties of atoms. From a practical point of view, they allow us to reduce the empiricism and improve the efficiency of computational models for vdW interactions.

[1] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)
[2] Jones *et al.*, Phys. Rev. B **87**, 144103 (2013)
[3] Fedorov *et al.*, Phys. Rev. Lett. **121**, 183401 (2018)

CPP 7.8 Mon 12:30 H9

impact of continuum electronic states on van der Waals dispersion interactions — •Mohammad Reza Karimpour, Dmitry Fedorov, and Alexandre Tkatchenko — University of Luxembourg, Luxembourg, Luxembourg

The ubiquitous van der Waals (vdW) forces play an important role for structure, stability, and dynamics of molecules and materials. Their description on atomistic level is important for molecular physics, crystal chemistry, surface science, structural biology, and pharmacy. To this end, the development of simple yet efficient models is of high importance. Normally, such models focus only on fluctuations to bound electron states, described via quantum harmonic oscillator potentials. However, the polarizability of real atomic and molecular systems has important contributions also from fluctuations to continuum states. To study their influence on the vdW dispersion interactions from a general point of view, here we consider models based on the Dirac delta-function potentials. In one-dimensional case, such a potential provides just one bound state whereas all excited states belong to the continuum electron spectrum. We apply both the atomistic method and the scattering picture representing the van der Waals and Casimir approaches for dispersion interactions, respectively. In the atomistic framework we compare our results to the ones of the quantum oscillator models. Within the other picture, we discuss an obtained new scaling law in comparison to the results known for excited atomic systems.

[1] Woods *et al.*, Rev. Mod. Phys. **88**, 045003 (2016)
[2] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)

CPP 7.9 Mon 12:45 H9

Relation between the van der Waals radius and higher-order atomic polarizabilities — •Ornella Vaccarelli, Dmitry Fedorov, and Alexandre Tkatchenko — University of Luxembourg, Luxembourg, Luxembourg

The atomic polarizabilities and van der Waals (vdW) radii describe the electronic and geometric aspects of the ubiquitous vdW interactions [1, 2], respectively. Normally, these quantities are assumed to be independent. Therefore, they are determined separately from each other. Based on the quantum Drude oscillator model [3], recently we revealed [4] a remarkable direct relationship between the vdW radius and the dipole polarizability. This provides a unified determination of the vdW radius for all chemical elements solely in terms of their dipole polarizabilities. In addition, further relations between the vdW radius $R_{\rm vdW}$ and higher-order atomic polarizabilities α_n $(n = 1, 2, ...)$ were found empirically. Here, we present a physical background for these results. The derivation of the corresponding scaling laws is performed by going beyond the dipole approximation for the Coulomb interaction to obtain higher-order contributions to attractive and repulsive forces acting on atoms in a vdW-bonded homonuclear dimer. We focus on the derivation of the proportionality constants C_n in the general relation $R_{\rm vdW}(\alpha_n) = C_n\ \alpha_n^{2/7(n+1)}$ unveiling their quantum nature.

[1] Woods *et al.*, Rev. Mod. Phys. **88**, 045003 (2016)
[2] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)
[3] Jones *et al.*, Phys. Rev. B **87**, 144103 (2013)
[4] Fedorov *et al.*, Phys. Rev. Lett. **121**, 183401 (2018)

CPP 8: Interfaces and Thin Films (joint session CPP/DY)

Time: Monday 15:00–17:15 Location: H14

CPP 8.1 Mon 15:00 H14

In situ GISAXS Investigations of Multi-responsive Block Copolymer Thin Films during Solvent Vapor Annealing — •Florian Jung[1], Panayiota A. Panteli[2], Detlef-M. Smilgies[3], Dorthe Posselt[4], Constantinos Tsitsilianis[5], Costas S. Patrickios[2], and Christine M. Papadakis[1] — [1]Physics Department, Soft Matter Group, Technical University of Munich, Garching, Germany — [2]Department of Chemistry, University of Cyprus, Nicosia, Cyprus — [3]Wilson Laboratory, Cornell University, Ithaca, USA — [4]Department of Science and Environment, Roskilde University, Roskilde, Denmark — [5]Department of Chemical Engineering, University of Patras, Patras, Greece

In the present work, we investigate the structure of a pH and temperature responsive, CBABC type pentablock terpolymer in thin films during solvent vapor annealing (SVA) using grazing-incidence small-angle X-ray scattering. The C end blocks are statistical copolymers of the hydrophobic n-BuMA and the thermoresponsive TEGMA, the B blocks are the weak cationic polyelectrolyte PDMAEMA and the A block is the hydrophilic PEG. Films were prepared by spin coating from aqueous solutions of different pH values. SVA experiments were carried out using both water and toluene as solvents. Films prepared at low pH feature a spherical morphology, and swell strongly in water, but only weakly in toluene vapor. At high pH, no structural features are observed, indicating the importance of ionization for microphase separation. During swelling in toluene, a morphology of small spheres is observed in the swollen state, while water has no noticeable effect.

CPP 8.2 Mon 15:15 H14

Competition of structural and electrostatic forces in colloidal dispersions confined between of two charged surfaces — •Michael Ludwig and Regine von Klitzing — Soft Matter at Interfaces, Department of Physics, Technische Universität Darmstadt

Structural forces can be observed when pure solvents and ionic liquids, as well as dispersions containing nanoparticles, micelles, polymers or polyelectrolytes are confined between two smooth surfaces into a thin liquid film. Upon surface-approach, liquid matter has to be depleted from the vicinity of the surfaces, altering the interactions between the surfaces.

The present study addresses structural forces across thin films of suspensions of nanoparticles (NP) confined between two charged surfaces measured with a colloidal-probe atomic force microscope (CP-AFM). Special attention is drawn to the transition from diluted to concentrated NP-packing and to the effect of the outer surface charge. An extended fitting procedure was introduced to accurately fit experimental data. The need of an additional repulsive contribution to the fitting formula will be discussed in terms of the DLVO-framework.

CPP 8.3 Mon 15:30 H14

Growth Kinetics and Molecular Mobility of Irreversibly Adsorbed Layers in Thin Films of P2VP and PVME — •Marcel Gawek, Sherif Madkour, Andreas Hertwig, 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 formed. These adsorbed layers have shown enormous potential for technological applications. Due to the hard accessibility of these layers, their growth kinetics and molecular dynamics are still not fully understood. Here, the irreversibly adsorbed layers of Poly(2-vinylpyridine) (P2VP) and Poly(vinyl methyl ether) (PVME) thin films are revealed by solvent-leaching experiments. 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) and spectroscopic ellipsometry. Additionally, the molecular mobility of the adsorbed layer is investigated with Broadband Dielectric Spectroscopy (BDS). A recently developed nanostructured capacitor (NSC) is employed to measure the adsorbed layers with a free surface layer depending on annealing and solvent-leaching time. The results are quantitatively compared and discussed with respect to recently published work.

CPP 8.4 Mon 15:45 H14

Enhanced protein adsorption near a phase transition — •Madeleine R. Fries[1], Daniel Stopper[1], Fajun Zhang[1], Robert M. J. Jacobs[2], Maximilian W. A. Skoda[3], Roland Roth[1], and Frank Schreiber[1] — [1]University of Tübingen, Germany — [2]University of Oxford, UK — [3]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 biomedicine. In particular, globular proteins tuned by multivalent ions give rise to a rich phase behavior including reentrant condensation and liquid-liquid phase separation (LLPS) through ion-bridges connecting individual proteins [1, 2]. Multivalent ions can be used not only to modify the bulk behaviour, but also the adsorption behaviour of proteins at the solid-liquid interface [3]. Here, we demonstrate experimentally that protein adsorption at attractive substrates can be enhanced significantly by approaching the LLPS regime through an increase in temperature or protein concentration, pointing towards the ability to control protein adsorption by means of suitably tailoring thermodynamic conditions. This is supported by theoretical calculations treating proteins as limited-valence (patchy) particles. These results could enable better biocompatibility in implants through guided protein-substrate interactions. [1] Zhang et al, PRL (2008); [2] Roosen-Runge et al, Sci. Rep. (2014); [3] Fries et al, PRL (2017)

15 min. break

CPP 8.5 Mon 16:15 H14

Templated electrodeposition of nanoscale semiconductors — •Li Shao[1], Andrew Hector[1], Philip Bartlett[1], Francis Sweeney[2], Samantha Soule[1], Richard Beanland[2], and Gilles Moehl[1] — [1]Chemistry, Southampton University, University Rd, SO17 1BJ, United Kingdom — [2]Department of Physics, University of Warwick, Coventry CV4 7AL

The Advanced Devices by ElectroPlaTing (ADEPT) project, an interdisciplinary research project funded by the EPSRC (EP/N035437/1), aims to develop new techniques and materials for thermoelectric devices, infrared detection, and phase change memory, by using electrodeposition methods. In previous work, Sn nanowires were deposited into mesoporous silica templates with pores of 1.5nm diameter.1 In this work, well-ordered mesoporous silica films with 3D pore structures were prepared by the evaporation-induced self-assembly (EISA) method. Using these silica films as templates, tellurium was deposited into the 3D pores. Grazing incidence small-angle X-ray scattering (GISAXS), scanning electron microscopy (SEM) and transmission electron microscopy (TEM) were used to characterize film nanostructures before and after electrodeposition. Programmes based on the distorted wave Born approximation (DWBA) were used for analysis and simulation of the 2D diffraction patterns from GISAXS. The patterns show that silica films with different structures including cubic, hexagonal and orthorhombic were synthesized. 1.*Philip N. Bartlett et al, Nano Lett. 2018, 18, 941*947. Type: Talk Topic: Thin films division Email: L.Shao@soton.ac.uk

CPP 8.6 Mon 16:30 H14

In-situ GISAXS during sputter deposition of metal nanolayers on functional polymer thin films for lithium-ion batteries — •Simon J. Schaper[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[4], 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 — [4]KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden

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. 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 and composites used in LIBs. Different polymer films are compared with respect to the metal layer growth.

CPP 8.7 Mon 16:45 H14

Using GISAXS to reveal spatial correlations in the electrochemical nucleation of gold particles — •Gilles Moehl, Philip Bartlett, and Andrew Hector — Chemistry, Southampton University, University Rd, SO17 1BJ, United Kingdom

Gilles E. Moehl, Philip N. Bartlett and Andrew L. 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. Electrochemical nucleation was generally described theoretically many years ago as a random process, which mainly depends on the deposition rate applied through the set current or potential, resulting in either instantaneous or progressive nucleation. Further development of theory and experiments has shown that the underlying process is just random, but that every newborn nucleus has the potential to influence the evolution of further nucleation steps. In this work, we show how grazing incidence small angle scattering can reveal spatial correlations in seemingly randomly arranged gold particles from electrolytic metal deposition.

CPP 8.8 Mon 17:00 H14

An Extended Transfer Matrix Approach to Calculate the Scattering of Light in an Interface Profile — •Reinhard Sigel — 83301 Traunreut

The transfer matrix method is a reliable work horse for the calculation of the reflection at an interface profile. In this contribution, the approach is extended by additional fluctuations $\Delta\varepsilon$ of the relative permittivity ε within the profile, which cause light scattering. For small amplitudes, such fluctuations can be treated within the first Born approximation. The incident light as well as the exit of the scattered light through the layered profile are handled by the transfer matrix method. Based on a model which yields the interface profile and the fluctuation amplitudes, the intensity and the polarization properties of the light scattered in any solid angle are predicted. Applications to grazing incidence small angle X-ray scattering (GISAXS), evanescent wave dynamic light scattering (EWDLS) and scattering ellipsometry are discussed.

CPP 9: Organic Electronics and Photovoltaics I - Charge Transport and Electronic Devices

Time: Monday 15:00–17:15 Location: H18

Invited Talk CPP 9.1 Mon 15:00 H18

Bulk Amounts of (6,5) Carbon Nanotubes for (Opto)- Electronic Devices — •Jana Zaumseil — Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany

Large volumes of highly purified dispersions of semiconducting (6,5) single-walled carbon nanotubes are readily available through polymer-wrapping and shear-force mixing. They enable the deposition (e.g. by aerosol jet printing) of semiconducting nanotube layers of variable thickness from sparse networks to 300 nm thick films with large optical density. These layers can be applied in lateral and vertical field-effect transistors with excellent device performance, but also as electrochromic filters, for organic light-emitting diodes in the near-infrared and photovoltaic cells. Here, we present examples of such applications and investigate the impact of novel n-dopants on nanotube networks, temperature-dependent charge transport and their optical properties at different charge carrier densities.

CPP 9.2 Mon 15:30 H18

The impact of energy barriers at grain boundaries on charge carrier motion in a high-mobility, electron-conductive organic semiconductor — Ilja Vladimirov[1], Michael Kühn[1], Thomas Gessner[1], Falk May[1], and •Thomas Weitz[2] — [1]BASF SE, Ludwigshafen, Germany — [2]AG Physics of Nanosystems, Faculty of Physics, LMU München, Germany

Using high-surface tension solvents allowed us to grow 3 * 10 nm thin, highly-crystalline films of a N,N*-di((S)-1-methylpentyl)-1,7(6)-dicyano-perylene-3,4:9,10-bis(dicarboximide) (PDI1MPCN2) at the liquid/air interface of a drying droplet [1]. We find, that charge carrier mobilities in these electron conductive films is as high as 4 cm*/Vs even for an only 3 nm thin PDI1MPCN2 film. Changing the solvent composition used for crystallization of our organic semiconductor also has allowed us to systematically tune the crystallinity and consequently the grain boundary density in thin films. From the temperature-dependent charge carrier mobility, we have extracted the density of states and compared it to Kinetic Monte Carlo simulations [2]. This combined theoretical and experimental approach has allowed us to identify, that it is rather the energetic barriers at grain boundaries than the usually identified traps that limit charge carrier motion. We also have revealed that the dipole moment of the PDI1MPCN2 is the cause for the energetic disorder at grain boundaries serving as clear guideline for future design of organic semiconductors with potentially no energetic barriers present at the grain boundaries. [1] Nano Lett. 18, 9, (2018) [2] Sci. Rep. 8, 14868, (2018)

CPP 9.3 Mon 15:45 H18

Electronic couplings in molecular crystals: Tight-Binding fits vs. cluster-based approaches — •Florian Mayer, Christian Winkler, and Egbert Zojer — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

The ever-growing interest in electronic properties of new materials triggers the development of new methodologies for their reliable description. For modelling charge-transport properties, theories span the full range from band transport via dynamic-disorder models to hopping approaches. For all these methods the electronic coupling between neighboring molecules is a crucial input. This quantity can be calculated with various approaches most of them relying on simulations of molecular dimers and small clusters. In contrast, the fitting of extended Tight-Binding models to full band structures allow the evaluation of intermolecular coupling, treating the molecules in their actual crystalline environments. In the present contribution, for the prototypical examples of pentacene and quinacridone, applying the above-mentioned complementary approaches, we discuss issues like next-nearest neighbor coupling, interference between different coupling directions for coherent transport, and how to deal with off-Gamma point band extrema. For non-periodic calculations we also present a new variant of the fragment orbital and electronic splitting method. The obtained results provide insight into the strengths and limitations of the various approaches and help to better understand electronic coupling in organic semiconductors.

15 min. break

CPP 9.4 Mon 16:15 H18

Finding the right building blocks for molecular optimization - Mining a database of organic semiconductors — •Christian Kunkel, Christoph Schober, Johannes T. Margraf, Karsten Reuter, and Harald Oberhofer — Chair for Theoretical Chemistry, Technical University Munich

Improving charge carrier mobilities of organic semiconductors is usually tackled by empirical structural tuning of a promising compound. Knowledge-based methods can greatly accelerate such local exploration by providing an overview of the problem-specific design space. Here, we provide such an overview for organic semiconductors, applying data mining strategies to an in-house database of >64.000 organic molecular crystals, annotated with charge-transport descriptors (electronic coupling and the reorganization energy) that are calculated from first principles. This database-screening recovers many known and well-performing materials, while also uncovering many more promising candidates, not yet considered for organic electronics applications. Analysing the design space regions in this dataset by a chemical space network hints at already explored or promising regions. We further derive general design principles by evaluating the performance of molecular scaffold and sidegroup clusters of compounds. For these, we find certain scaffolds (sidegroups) to consistently improve charge-transport properties. Functionalizing promising scaffolds with favorable sidegroups then results in molecular crystals with improved charge-transport properties, highlighting the usefulness of data-based approaches for a targeted design of organic electronics materials.

CPP 9.5 Mon 16:30 H18

Calculating electron - phonon coupling with density functional theory to describe polaron dynamics — •Oliver Stauffert[1], Roman Krems[2], Mona Berciu[2], and Michael Walter[1] — [1]Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany — [2]University of British Columbia Faculty of Science

In order to investigate on novel materials, we describe electronic structures for organic molecules, with density functional theory (DFT). Hereby we are especially interested in couplinging of electronic and nuclear degrees of freedom to investigate polaron phenomena. These have been proposed based on the Su-Schrieffer-Heeger (SSH) Hamiltonion and might lead to superconducting states. We use DFT calculations to obtain the SSH pa- rameters of polyacetylene and its derivatives in order to explore a set of possible materials with strong electron-phonon coupling. Our results predict an increase of the coupling parameter through stretching of the chain or by substitution of the hydrogens by other side groups. With the new insight gained in the electron phonon coupling within these simple chains, one might improve the understanding of polarons in more complex materials and take a step towards the direction of high temperature superconductors.

CPP 9.6 Mon 16:45 H18

Why are charge-carrier mobilities in organic semiconductors typically low? The instructive case of quinacridone — •Christian Winkler, Florian Mayer, Oliver T. Hofmann, Gernot J. Kraberger, and Egbert Zojer — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz

In this contribution, using first principles approaches, we study the interplay between transport relevant parameters, total energy, and crystal structure by using the instructive example of quinacridone. For this material, one finds three polymorphs with fundamentally different packing motifs. Additionally, based on the α-polymorph, an artificial coplanar quinacridone crystal can be constructed. The latter allows correlating electronic properties like transfer integrals t and effective masses m* with the total energy of the crystal. This yields a clear correlation between energetic minima and poor transport parameters suggesting that in π-stacked systems Pauli-exchange repulsion triggers a shift between neighboring molecules such that the inter-molecular electronic coupling is minimized. Possible strategies for overcoming this negative correlation can be derived from the properties of β- and γ-quinacridone, where larger transfer integrals result from modified van der Waals interactions and complex H-bonding networks.

CPP 9.7 Mon 17:00 H18

Hopping-approach in organic semiconductors: mode-resolved vibrations and improved time-consistency — •Sebastian Hutsch and Frank Ortmann — Center for Advancing Electronics Dresden, Technische Universität Dresden, Germany

The charge carrier mobilities of different organic semiconductor systems can span several orders of magnitude, making the precise description of different transport regimes necessary. When a localization of the charge carrier is expected, e.g. due to a strong electron-phonon coupling, the transport is assumed to be hopping-like. This regime is usually treated within the Marcus theory or Levich-Jortner theory, which however approximate the rich vibrational spectrum of organic semiconductors, for example in the high-temperature limit. We are presenting a hopping-approach that overcomes these limitations by treating the intramolecular modes in a mode-resolved fashion. This refined approach further allows to individually treat each mode statically or dynamically in the calculation of the hopping-rate, i.e. ensure the time-consistency in the treatment of the vibrations.

CPP 10: Crystallization, Nucleation and Self-assembly I

Time: Monday 15:00–17:30 Location: H13

CPP 10.1 Mon 15:00 H13

The Underestimated Effect of Intracrystalline Chain Dynamics on the Morphology and Stability of Semicrystalline Polymers — •Martha Schulz, Anne Seidlitz, Ricardo Kurz, Ruth Bärenwald, Albrecht Petzold, Kay Saalwächter, and Thomas Thurn-Albrecht — Martin-Luther-Universität Halle-Wittenberg

Some polymers show translational motion of the chains in crystallites - the α_c-relaxation. Although it was recognized early by BOYD that α_c-mobile polymers have a higher crystallinity than crystal-fixed polymers, the relaxation process has been ignored in most crystallization models. We show that the α_c-relaxation has a strong influence on the crystallization process, changing morphology and stability of the semicrystalline structure. Using SAXS, we compare structural characteristics for PEO (α_c -mobile) and PCL (crystal-fixed) after isothermal crystallization and during heating. With NMR we can estimate the timescale of the α_c-relaxation depending on T_c. A direct comparison points out fundamental differences: PCL shows marginally stable lamellae with a narrow thickness distribution, starting to reorganize for $T > T_c$. In contrast, PEO shows a well-defined, narrowly distributed amorphous thickness da and a broad thickness distribution of the lamellae. For $T > T_c$, the lamellae are stable over a wide range. We hypothesize that due to the α_c-relaxation, the lamellae thicken directly behind the growth front up to a minimal da. This is supported by NMR-results: At high T_c the α_c-relaxation is fast enough to enable crystal reorganization to take place in a narrow zone directly behind the growth front.

Schulz, M.; Macromolecules 51, 8377 (2018)

CPP 10.2 Mon 15:15 H13

Combining Infrared Micro-Spectroscopy and Fast Scanning Chip Calorimetry to unravel homogeneous nucleation and crystallization in poly(amide-6-6) — Wilhelm Kossack[1], Evgeny Zhuravlev[2], Rustem Andrianov[3], Christoph Schick[2,3], and •Friedrich Kremer[1] — [1]University Leipzig, molecular physics, Linnestr. 5, Leipzig, Germany — [2]Institute of Physics and Competence Centre CALOR°, University of Rostock, Albert-Einstein-Str. 23-24, 18051 Rostock, Germany — [3]Institute of Chemistry, Kazan Federal University, 18 Kremlyovskaya Street, Kazan 420008, Russian Federation

A combination of Infrared micro-spectroscopy and Fast Scanning calorimetry is used for a simultaneous measurement of moiety specific IR-absorption and heat capacity in the super-cooled amorphous melt of poly(amide-6-6). The temporal evolution of both quantities is recorded depending on temperature and time to unravel the microscopic, moiety-specific mechanism of homogeneous nucleation. The IR results reveal a continuous increase of bands related to the crystalline phase on expense of the amorphous phase. In agreement with classical nucleation theory, first experiments do not reveal a moiety-specific interaction during homogeneous nucleation. Furthermore both, IR-signature and calorimetric crystallinity and nuclei densities follow similar kinetics. In summary, no evidence is found that homogeneous nuclei and early crystals differ qualitatively on the level of a unit cell from well grown lamellae. Based on these experiments an experimentally based estimate of the size of homogeneous nuclei is possible.

CPP 10.3 Mon 15:30 H13

Visualization of Polymer Crystallization by a Combination of Atomic Force Microscopy and Fast Scanning Calorimetry — •Rui Zhang[1,2], Evgeny Zhuravlev[1,2], and Christoph Schick[1,2,3] — [1]Institute of Physics, University of Rostock, Albert-Einstein-Str. 23-24, 18051 Rostock, Germany — [2]Competence Centre CALOR, Faculty of Interdisciplinary Research, University of Rostock, Albert-Einstein-Str. 25, 18051 Rostock, Germany — [3]Kazan Federal University, 18 Kremlyovskaya street, Kazan 420008, Russian Federation

Atomic force microscopy (AFM) can show the morphology of the crystal structures of semi-crystallized polymers with resolution from micrometers to nanometers scales. Meanwhile, fast scanning calorimetry (FSC) can treat the polymer sample heating and cooling until 1,000,000 K/s, which enables to achieve expected annealing temperature without re-crystallization processes. By combining with AFM and FSC (AFM-FSC), the scanner of AFM plays as the chip-sensor holder and enables the FSC to be directly measured on the AFM without changes of the sensor. By this way, the polymer sample can be annealed at expected temperature and time and these formed crystals structures can be accessed to AFM after fast cooling to environmental temperature. Some results will be reported in presentation.

CPP 10.4 Mon 15:45 H13

Visualization of Dynamic Processes with Video-Rate Atomic Force Microscopy — •Ted Limpoco, Mario Viani, and Marta Kocun — Asylum Research, an Oxford Instruments company, 6310 Hollister Ave, Goleta, U.S.A.

Atomic Force Microscopy (AFM) is a unique and powerful tool for measuring structural, mechanical, and electrical properties of materials at the nanometer scale. A limitation of conventional AFM is that it is a slow technique, with image acquisition times on the order of minutes. The recent introduction of a practical video-rate AFM has improved imaging speeds and makes it now possible to capture movies with a temporal resolution better than a second. This presentation will cover some recent results taken via video-rate AFM, including the real-time self-assembly of collagen into fibrils and the migration of surfactant micelles on graphite. Additionally, we will discuss related results such as the melting/re-crystallization of polymers and consider future research opportunities that might be enabled by this technology.

15 min. break

CPP 10.5 Mon 16:15 H13

Polymorphism and crystal stability of syndiotactic polystyrene from multiscale simulations — •Chan Liu, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Syndiotactic polystyrene (sPS) exhibits complex polymorphic behavior upon crystallization. Computational modeling of polymer crystallization has remained a challenging task because the relevant processes are slow on the molecular time scale. In previous work, we have found that our coarse-grained (CG) model of sPS significantly speed up the simulations, while stabilizing the main polymorphs α and β, observed experimentally. However, to study the stability of polymorphs, we require reasonably larger system and more advanced enhanced-sampling methods, such as Metadynamics. Furthermore, we rely on Markov state models to gain insight into the kinetics of interconversion between polymorphs and to verify the convergence of Metadynamics.

CPP 10.6 Mon 16:30 H13

Thermodynamic Principles of Prefreezing as a First-Order Transition — •Oleksandr Dolynchuk, Muhammad Tariq, and Thomas Thurn-Albrecht — Experimental Polymer Physics, Institute of Physics, Martin Luther University Halle-Wittenberg, Germany

Crystallization of liquids on a solid surface can be initiated by either

heterogeneous nucleation or prefreezing. The latter phenomenon is the crystalline layer formation at an interface to a solid substrate at a temperature higher than that of a bulk crystal. As it was recently determined, prefreezing is a first-order transition, since the formation of the crystalline phase is abrupt and reversible.
Here, we present a phenomenological theory of prefreezing and analyze such equilibrium properties as the temperature dependent thickness of the prefrozen layer, the maximum temperature range of prefreezing T_{max}, and the mesoscopic jump of thickness during crystallization or melting. The theory provides a clear first-principles explanation of the first-order nature of prefreezing and defines the corresponding transition temperature T_{max} as a function of the interfacial free energies. As shown, it is the difference of the interfacial energies that controls T_{max} and serves as a driving force for prefreezing. The theoretical outcomes are applied to quantify the recent experimental results for poly(ϵ-caprolactone) crystallized on graphite via prefreezing.

CPP 10.7 Mon 16:45 H13

Small polyethylene systems: aggregation and low tempereture configurations — •Timur Shakirov and Wolfgang Paul — Institute of Physics, University of Halle, Halle, Germany

The phase behavior of dilute solutions of polyethylene chains has been under investigation for many decades. But investigation of the equilibrium structures of single alkane chains and their aggregation have been addressed in far less detail. We present here results of a Wang-Landau-type Monte Carlo simulation [1,2], 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 [3]. Simulation results for deep-energy (or equivalently low temperature) states demonstrate a set of various ground-state configurations: from stretched configurations of short chains to a helix-like structures reeled round one of the chains. Aggregates of a few chains demonstrate complex temperature 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 number of monomers. However, with increasing chain length, single chain and aggregate morphologies become more similar.

[1] F. Liang, C. Liu, R. J Carroll, J. Am. Stat. Assoc. 2007, 102, 305-320.

[2] T. Shakirov, Comp. Phys. Commun. 228 (2018): 38-43.

[3] W. Paul, D. Y. Yoon, and G. D. Smith, J. Chem. Phys. 103 (1995) 1702-1709.

CPP 10.8 Mon 17:00 H13

Steric and Hydrophobic Interactions Determine Self-assembly of Supramolecular Nanorods — •Saikat Chakraborty[1], Christian Berac[2], Pol Besenius[2], and Thomas Speck[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 7-9, 55128 Mainz, Germany. — [2]Institut für Organische Chemie, Johannes Gutenberg-Universität Mainz, Duesbergweg 10-14, 55128 Mainz, Germany.

C_3-symmetric amphiphilic peptides have been successfully applied for the construction of supramolecular aggregates of defined size and shape. These compounds typically contain a hydrophobic core and three amphiphilic arms. In water, due to combined effects of hydrphobic interactions, hydrogen bonding and shielding effects of flexible hydrophilic chains, the monomers stack over one another to form one-dimensional nanorods. We present a minimal model for efficient simulations of such unidirectional self-assembly without the requirement of an explicit solvent. Composites of the monomers interact among themselves via simple pair potentials to invoke hydrophobic and steric effects. We show that these factors are sufficient to obtain self-assembly of the monomers into elongated, defect-free, rod-like structures from highly dilute, disordered initial state. This assembly kinetics have been linked to the microscopic processes governing the polymerization. The understanding thus obtained, has been used to draw comparison with the experiments. Further, study of the morphology of the nanorods reveals that beyond a threshold value of hydrophobic interactions among these achiral building blocks, there is a transition to helical structure.

CPP 10.9 Mon 17:15 H13

Fabrication of polymeric Janus nanoparticles and their behavior at liquid-liquid interfaces - a simulation study — •Tatiana Morozova and Arash Nikoubashman — Johannes Gutenberg University, Mainz,Germany

Polymeric nanoparticles (NPs) are promising candidates for a wide range of applications such as colloidal self-assembly and targeted therapeutics. Flash Nanoprecipitation (FNP) is a scalable technique for fabricating monodisperse polymeric NPs through rapid micromixing of a polymer solution with a miscible poor solvent. In this simulation work, we are studying the fabrication of Janus NPs with one solvophilic and one solvophobic hemisphere, and their behavior at liquid-liquid interfaces. We performed coarse-grained molecular dynamics simulations of the FNP process using two types of solvophobic homopolymers and one type of amphiphilic blockcopolymers (BCPs). We systematically investigated the influence of the composition and concentration of the BCPs on the resulting NP morphology. We determined the parameter space where amphiphilic Janus or core-shell NPs can be formed, and studied the conformation of BCPs at the NPs surface. Finally, in order to test the potential of these NPs as colloidal stabilizing agents, we placed them at the interface between two immiscible liquids. Indeed, we observed a significant reduction of the surface tension for both core-shell and Janus NPs.

CPP 11: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods

Time: Monday 15:00–16:00 Location: H8

CPP 11.1 Mon 15:00 H8

GISANS sample environment for the investigation of thin polymer films — •Tobias Widmann[1], Lucas Kreuzer[1], Nuri Hohn[1], Kun Wang[1], Gaetano Mangiapia[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, 85748 Garching — [3]Bielefeld University, Physical and Biophysical Chemistry, 33615 Bielefeld

The investigation of thin polymer films with neutrons allows a non-destructive probe on their structure and composition. In the framework of the FlexiProb project, which plans an interchangeable sample environment for different neutron experiments at the European spallation source (ESS), we designed a setup for grazing incidence small angle neutron scattering (GISANS). The new sample chamber offers a wide range of adjustable relative humidity with fast switching times. Moreover, a homogeneous heat distribution and reduced condensation of the humid air is realized by a spherical design with fluidic channels inside the chamber walls. A separate gas-mixing and air-flow setup, gives precise control over the air conditions inside the chamber. To demonstrate its options, thin microgel films constituted of thermoresponsive NIPAM with N,N'-methylenebisacrylamide as cross-linkers are placed inside and humidified from 0 to 100 %RH and vice versa. The film response is analyzed with time-of-flight GISANS in order to observe structural changes in the films over the course of the humidification.

CPP 11.2 Mon 15:15 H8

Development of a Sample Environment for in-situ Dynamic Light Scattering in Combination with Small Angle Neutron Scattering for the Investigation of Soft Matter at the European Spallation Source ESS — •Andreas Schmid[1], Sebastian Jaksch[2], Henrich Frielinghaus[2], Tobias Schrader[2], Harald Schneider[3], and Thomas Hellweg[1] — [1]Physical and Biophysical Chemistry, Bielefeld University, Bielefeld, Germany — [2]Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ, Garching, Germany — [3]Scientific Activities Division, FLUCO Platform, European Spallation Source ERIC, Lund, Sweden

The most brilliant and most powerful neutron source in the world, the European Spallation Source ESS, is currently built in Lund. In our project FlexiProb we developed three sample environments for the investigation of soft matter to maximize the potential of the ESS with regard to the very high neutron flux. These are sample environments for small angle neutron scattering (SANS) with in-situ dynamic light scattering (DLS), under gracing incidence (GISANS) and on free-standing liquid films and foams. All sample environments are built on an universal carrier system to ensure a high repeatability and flexibility as well as a minimum switching time between different sample environments. The DLS/SANS module developed in our subproject provides additional control parameters, e.g., the sample stability during the SANS measurements. We developed a special sample holder for about 40 samples which allows the simultaneous measurement of SANS and DLS at two different scattering angles and a precise temperature control.

CPP 11.3 Mon 15:30 H8

Container-free sample environment for neutron scattering — •Sebastian W. Krauss[1], Ralf Schweins[2], Andreas Magerl[3], and Mirijam Zobel[1] — [1]University Bayreuth, Bayreuth, Germany — [2]Institut Laue Langevin, Grenoble, France — [3]Friedrich-Alexander-University Erlangen-Nuremberg, Erlangen, Germany

In-situ small angle X-ray and neutron scattering (SAXS / SANS) provide valuable insights into soft matter systems, such as micelles, biological macromolecules or nanoparticle (NP) formation. For SAXS free-jet setups are established, but the counterpart for SANS was missing, as SANS requires large sample cross sections[1]. Here, we introduce a novel free-film setup, where the neutrons only penetrate a flowing liquid film optimized to a sample area of 7x10 mm^2 with a typical film thickness of 0.5 mm as determined from the incoherent scattering of the film. In order to suppress H/D-exchange from the humidity in the air for the operation of the setup with deuterated solvents, we jacketed the setup in a containment filled with Helium. To validate the H/D-ratio over time, three independent methods have been used: IR, gravimetry, incoherent neutron scattering. The main benefit of the free-film is the reduction of the background scattering by 37 % in comparison to measurements in a standard Hellma cell as typically used for SANS. Furthermore, we showcase the setup for the formation of EDTA-capped CdS nanoparticles, in order to investigate the role of the weakly scattering EDTA ligand shell in the nucleation process, having been inaccessible so far.

[1] Lopez, C. G., (2018). J Appl Crystallogr 51, 570-583.

CPP 11.4 Mon 15:45 H8

Gold-labels Enhance Small-angle X-ray Scattering Measurements — •Jan Lipfert — LMU Munich

SAXS is a powerful tool to probe the structure, interactions and dynamics of biological macromolecules and their complexes in free solution, under virtually arbitrary solution conditions. However, the information content in traditional SAXS measurements is limited, making it impossible to obtain atomic resolution structures from SAXS data alone. To enhance the information content available from standard biological SAXS measurements, we use small (~1.4 nm diameter) gold nanocrystals. The gold nanoparticles can be site-specifically attached to DNA, RNA, and proteins, provide very high scattering contrast in aqueous buffer, and are well suited for ASAXS experiments. We have recently demonstrated two different and complementary schemes to apply gold labels in biological SAXS measurements: As molecular distances rules in ASAXS measurements [1] and as fiducial markers in standard biological SAXS measurements to provide a sequence-to-low resolutions structure map [2]. Here, I will discuss the possibilities provided by these labelling schemes and given an outlook on how they will be able to provide novel insights into the structure and dynamics of polymers and biological macromolecules in solution. [1] T. Zettl et al., Nano Letters (2016) 16:5353-7. [2] T. Zettl et al., Science Advances (2018) 4:eaar4418.

CPP 12: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge II (joint session O/TT/DS/CPP)

Time: Monday 15:00–17:30 Location: H9

CPP 12.1 Mon 15:00 H9

Influence of structural deformations on the applicability of the Tamm-Dancoff approximation for 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 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 small organic molecules [1]. In this talk we discuss the applicability of the TDA for molecules of different sizes and show the transition between the two regimes. We then discuss how the applicability is influenced by deformations of the molecules, in particular by the related conjugation length of the π-system.

[1] B. Baumeier et al., J. Chem. Theory Comput. **8**, 997 (2012)

CPP 12.2 Mon 15:15 H9

Momentum-Resolved Electron Energy-Loss Spectroscopy in Oxides from Many-Body Perturbation Theory — •Christian Vorwerk[1,2], Caterina Cocchi[1,2], and Claudia Draxl[1,2] — [1]Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]European Theoretical Spectroscopy Facility

Electron energy-loss spectroscopy (EELS) is a powerful tool to investigate the local electronic and structural properties of crystalline materials. The accurate determination of these spectra from first principles requires a reliable description of the electron-hole interaction, screened by the surrounding many-electron system. We perform *ab initio* many-body perturbation theory calculations of EELS through the solution of the Bethe-Salpeter equation (BSE), including the screened non-local interaction between electron and hole. Employing an implementation in the all-electron full-potential package `exciting`, we show results for a wide range of energy loss, from the optical to the hard x-ray region. We study EELS at finite momentum loss $\mathbf{q}$, from small $\mathbf{q}$ close to the dipole limit to large $\mathbf{q}$ well beyond the first Brillouin zone. This momentum resolution of EELS reveals dipole-forbidden excitations that are invisible in absorption spectroscopy. Our calculations also yield insight into the excitonic dispersion, *i.e.* the excitonic bandstructure. We discuss the effects of momentum loss in the EELS spectra of oxide materials, including CaO, CeO$_2$, and the wide-gap transparent oxide Ga$_2$O$_3$, considering both the optical and x-ray energy-loss range.

CPP 12.3 Mon 15:30 H9

Electron-magnon scattering in elementary ferromagnets from first principles: implementation and results — •Christoph Friedrich, Mathias C.T.D. Müller, and Stefan Blügel — Peter Grünberg Institut and Institute of Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Propagating electrons and holes can scatter with spin fluctuations and form quasiparticles as a result or more complex many-body states. To calculate this effect, a $\mathbf{k}$-dependent self-energy describing the scattering of electrons and magnons is constructed from the solution of a Bethe-Salpeter equation for the T matrix. Partial self-consistency is achieved by the alignment of the chemical potentials. We discuss details of the implementation and illustrative results. The renormalized electronic band structures exhibit strong spin-dependent lifetime effects close to the Fermi energy, which are strongest in Fe. The renormalization gives rise to a band anomaly at large binding energies in iron, which results from a coupling of the quasihole with Stoner excitations.

CPP 12.4 Mon 15:45 H9

Dielectric function of homogeneous electron gas from Bethe-Salpeter equation — •Jaakko Koskelo[1,2], Martin Panholzer[2,3], Lucia Reining[1,2], and Matteo Gatti[1,2,4] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA, Université Paris-Saclay, F-91128 Palaiseau, France — [2]ETSF — [3]Institute for Theoretical Physics, Johannes Kepler University, Linz, Austria — [4]Synchrotron SOLEIL, France

The homogeneous electron gas (HEG) is one of the most important model systems in condensed matter physics, and it has been subject of a great number of studies. Some properties of HEG such as total energy and static correlation functions can be obtained from quantum Monte Carlo simulations with great accuracy, but for dynamical correlation functions only very few results are available.

Methods based on the Bethe-Salpeter equation (BSE) have been very succesful in semiconductors and insulators, but metals have been less studied. In this contribution, we use the BSE in its standard approximations, including a statically screened electron-hole interaction, to study the dielectric function of HEG. We find significant differences in static screening and spectra compared to other approaches. In particular, the BSE in its current approximations fails to reproduce the negative static screening in the low-density HEG, which is related to a so-called ghost exciton. We also use the time-dependent mean-density approximation [1] in order to compare our results to experimental loss spectra of sodium.

[1] M. Panholzer et al, Phys. Rev. Lett. **120**, 166402 (2018).

CPP 12.5 Mon 16:00 H9

DFT study of electronic and optical properties of SrTiO$_{3-\delta}$ 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.

The electronic and optical properties of SrTiO$_3$ (STO), a perovskite material of key importance in the field of oxide electronics, are explored in the framework of density functional theory including many-body effects within the GW approximation and excitonic corrections by solving the Bethe-Salpeter equation (BSE). We further analyse the origin of the strong excitonic effects, in particular a peak at ≈6.5 eV, by decomposing the BSE eigenvectors obtained from GW+BSE to extract the leading electron-hole pair contribution for the particular BSE eigenstate following the approach of Bokdam *et al.* [Scientific Reports 6, 28618 (2016)]. Alternatively, we use the model-BSE (mBSE) which utilises a parametrised analytical model for the static screening. For STO, the mBSE spectrum closely reproduces the one from GW+BSE, which allows to reduce the computational effort by circumventing the intermediate time-consuming GW step. We further proceed to describe the effect of oxygen defects on the electronic and optical properties in STO.

Funding by DFG- SFB1242, project C02 is gratefully acknowledged.

CPP 12.6 Mon 16:15 H9

Second-order Møller-Plesset perturbation theory and beyond for the band gap and single-particle excitations of solids — •Maria Dragoumi[1], Sergey V. Levchenko[2,1,3], Igor Ying Zhang[4,1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, DE — [2]Skolkovo Innovation Center, Moscow, RU — [3]NUST MISIS, Moscow, RU — [4]Fudan University, Shanghai, CN

Calculations of the fundamental band-gap and the low-energy excitations of solids are still a challenge for electronic-structure theory. The computationally efficient Kohn-Sham (KS) density functional theory (DFT) with the widely used local or semi-local approximations provides a KS band gap which is much smaller than the fundamental gap. Many-body perturbation theory, on the other hand, addresses the fundamental gap directly. We present here an efficient scalable implementation of Møller-Plesset second order perturbation theory (MP2) for quasi-particle energies [1,2]. By solving the Dyson equation of the single-particle Green's function, considering self-energy up to second order, we go beyond MP2. The new approach shows a competitive or even superior performance in comparison to the current state-of-the-art methods such as hybrid functionals and *GW* approximation, where second order exchange is missing. We present numerical results for the band-gap of a wide range of semiconductors and insulators.

[1] J. Sun and R. J. Bartlett, J. Chem. Phys. 104, 8553 (1996).
[2] A. Grüneis, et.al, J. Chem. Phys. 133, 074107 (2010).

CPP 12.7 Mon 16:30 H9

Accelerating *GW* Calculations within the LAPW Framework — •Sven Lubeck, Andris Gulans, and Claudia Draxl — Humboldt-Universität zu Berlin, Germany

The *GW* approach of many-body perturbation theory is an indispensable method for calculating the electronic band structure of solids. Its implementation in computer programs using the linearized augmented plane-wave + local orbital (LAPW+LO) method allows for obtaining numerically precise results. Unfortunately, high precision comes at the price of a large number of LAPWs and LOs. In this work, we accelerate *GW* calculations by optimizing the use of LAPWs and LOs in the computer package `exciting` [1]. On the one hand, we introduce a systematic way of obtaining a minimal set of LOs. On the other hand, we perform a basis transformation from the plane-wave part of the LAPWs to different types of basis functions, exploring the efficiency of numeric atom-centered orbitals, Gaussian type orbitals, and Kohn-Sham orbitals. Presenting band gaps of two exemplary materials, zincblende ZnO and hexagonal monolayer BN, we illustrate that our optimization schemes reduce the computational cost down to values as low as 15% without compromising the precision.

[1] A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti, S. Sagmeister, U. Werner, and C. Draxl, J. Phys.: Condens. Matter **26**, 363202 (2014).

CPP 12.8 Mon 16:45 H9

Ab-initio description of transient ion formation of NO on Au(111) — Daniel Corken, Nicholas D. M. Hine, and •Reinhard J. Maurer — Departments of Physics and Chemistry, University of Warwick, United Kingdom

Gaining a fundamental understanding of the interactions of molecules on metal surfaces is essential for the development of novel heterogeneous catalysts. An interesting feature of gas-surface reactions at metal surfaces is that the Born-Oppenheimer approximation breaks down. Vibrationally excited and translationally hot molecules can transfer energy to the electrons of a metal via excitation of electron-hole pairs (EHP). In case of NO on Au(111), [1] this nonadiabatic energy loss is believed to stem from the transient generation of charged ion species at the surface. A computationally feasible and accurate description of such a molecule-metal charge-transfer state represents a challenge and several methods have been proposed. Upon a review of existing experimental evidence, we will present our approach to this problem. We use linear expansion-Delta-Self-Consistent-Field Density Functional Theory (leΔSCF-DFT) [2] to model the anionic resonance of NO on Au(111). The leΔSCF-DFT method enforces the electronic configuration of reference molecular states while solving the Kohn-Sham equations self-consistently. By comparison to experiment and other models, we asses the methods' ability to describe the ground- and excited-states during molecular scattering. We further explore avenues to extract nonadiabatic couplings and to construct model Hamiltonians based on this method. [1] JCP 130, 174716, [2] JCP 139, 014708;

CPP 12.9 Mon 17:00 H9

Luminescence of β-SiAlON:Eu^{2+} phosphors: DFT study — •Saleem Ayaz Khan[1], Ondrej Sipr[1], Robin Niklaus[2], Wolfgang Schnick[2], and Jan Minar[1] — [1]University of West Bohemia, Pilsen, Czech Republic — [2]LMU Munich, Germany

Highly efficient phosphor-converted light-emitting diodes (pc-LEDs)are popular in lighting and high-tech electronics applications[1]. Among them β-SiAlON:Eu^{2+} stands out as a promising narrow-band green phosphor for white-LEDs applications exhibiting good thermal and chemical stabilities. Photoluminescent properties of this material can be tuned by introducing the disorder at various sublattices. To understand the mechanism behind this effect, we performed a systematic study of electronic structure and photoluminescence properties of β-SiAlON:Eu^{2+}. The calculations were done within the *ab-initio* fully relativistic full-potential framework. The disorder was treated by employing both the supercell approach and the coherent potential approximation (CPA). The Stokes shifts were calculated from differences of total energies of the ground and excited states of β-SiAlON:Eu^{2+}. The main focus is on monitoring how the Al and O content and Eu^{2+} activator concentrations influence the local β-Si3N4 electronic structure and how this may be used to tune photoluminescence properties.

[1] Z. Wang, W. Ye, Iek-H. Chu, and S. P. Ong, Chem. Mater., **28**, 8622 (2016).

CPP 12.10 Mon 17:15 H9

Spin fluctuations in itinerant ferromagnets: Computing the dynamic transverse spin susceptibility with TDDFT and PAW — •Thorbjørn Skovhus and Thomas Olsen — Technical University of Denmark

We present a numerical scheme for computing the dynamic transverse spin susceptibility using time-dependent density functional theory which allows us to study magnons in itinerant ferromagnets. The scheme is based on a real-space grid implementation of the projected augmented wave method and use a simple plane wave representation of the response function. Employing the adiabatic local density approximation for the exchange-correlation kernel, calculations of the magnon spectra in bulk transition metals iron and nickel are presented. In the context of the present implementation, the influence from the choice of numerical scheme on the violation of the Goldstone theorem is investigated.

CPP 13: Membranes and Vesicles II (joint session BP/CPP)

Time: Monday 15:00–16:15 Location: H10

CPP 13.1 Mon 15:00 H10

Screening of small molecules with bilayer-modifying properties using coarse-grained simulations — •Alessia Centi, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Small molecules, including alcohols and anesthetics, can alter the lateral organization of plasma membranes by preferentially partitioning between domains, thereby affecting lipid bilayer properties and stability. Although lipid segregation is key to many biological processes, precise understanding of the physical and chemical properties governing membrane phase behaviour is still lacking. Gaining more fundamental insight into the underlying mechanism is pivotal for developing enhanced drugs that can act through targeted domain phase separation.

In this work, we employ coarse-grained simulations based on the MARTINI force field [1] as a screening tool to identify compounds which can affect phase separation in model membranes. Hence, our approach based on a combination of molecular dynamics simulations and potential of mean force calculations, provides a rapid and affordable platform for gaining a better understanding of the driving forces of lipid domain stabilisation/destabilisation.

[1] S. J. Marrink, et al. Journal of Physical Chemistry vol. 111 p. 7812-7824, 2007.

CPP 13.2 Mon 15:15 H10

Drug-membrane permeability across chemical space — •Roberto Menichetti, Kiran H. Kanekal, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Unraveling the link between the chemical structure of a small drug-like molecule and its rate of passive permeation across a lipid membrane is of fundamental importance for pharmaceutical application. However, the elucidation of a structure-permeability relationship in terms of few molecular descriptors has been so far hampered by the overwhelming number of possible compounds. In this work, we reduce a priori the size of chemical space by relying on physics-based coarse-grained models, and perform high-throughput coarse-grained simulations (HTCG) to cover a subset of chemical space both efficiently and broadly. This comprehensive exploration allows us to derive a smooth surface relating the permeability of a compound to two simple molecular properties—the bulk partitioning free energy and acid dissociation constant. By projecting HTCG predictions back to atomistic resolution, we provide an estimate of the permeability coefficient for more than 500,000 small molecules in the range $30-160$ Da. Our large scale analysis establishes a clear connection between specific functional groups and the resulting permeability, enabling for the first time inverse molecular design. This study further highlights that favoring the incorporation of certain groups will reduce the range of accessible permeabilities, thus affecting bioavailability.

[1] R. Menichetti, K. H. Kanekal, and T. Bereau, arXiv preprint arXiv:1805.10158 (2018).

CPP 13.3 Mon 15:30 H10

X-Ray Reflectivity Investigation of Structure and Kinetics of Photoswitchable Lipid Monolayers — •Jonas Erik Warias[1], Svenja Carolin Hövelmann[1], Franziska Reise[2], Andrea Sartori[1], Rajendra Prasad Giri[1], Chen Shen[3], Thisbe Lindhorst[2], Olaf Magnus Magnussen[1], and Bridget Mary Murphy[1,4] — [1]Institut für Experimentelle und Angewandte Physik, University of Kiel, Germany — [2]Otto Diels-Institut für Organische Chemie, University of Kiel, Germany — [3]Deutsches Elektronen Synchrotron, Hamburg, Germany — [4]Ruprecht Heansel Laboratory, University of Kiel, Germany

The mechanical and dynamic properties of phospholipid membranes are of importance for biological functions, such as switching of embedded proteins and cell transportation. In order to investigate these properties we study model systems in which amphiphilic photoswitchable molecules are integrated into Langmuir films of phospholipids. We have modified glycolipids to contain an azobenzene photoswitch between the chain and the head group and successfully embedded those in a monolayer of dipalmitoylphosphatidylcholine (DPPC). This allows us to reversibly change the azobenzene-glycolipid orientation between trans- and cis-conformation by illumination with UV and blue light. We have followed the structural changes in this model membrane and the switching kinetics of the system with Langmuir isotherms and in situ X-ray reflectivity at the LISA diffractometer P08, PETRA III. Strong changes in membrane conformation upon switching have been observed and an additional phase transition has been discovered.

CPP 13.4 Mon 15:45 H10

On the propagation of acoustic waves along the membrane based on the thermodynamic state of the interface — •Kevin Kang and Matthias Schneider — Technische Universität Dortmund

Biological membranes form hydrated, quasi-2D elastic interfaces, and it has been proposed that acoustic waves propagating along the membrane play a fundamental role in biological communication. Here we investigate whether thermodynamic principles can be applied on interfaces to study mechanical signaling along membranes. Using fluorescent probes embedded on an lipid monolayer assembled at the air-water interface, we excite the monolayer and measure the acoustic waves propagating along the membrane using FRET. We find that stimulation near the phase transition region of the state diagram (liquid-expanded/liquid condensed) can generate all-or-none type pulse, and the threshold behavior and the pulse shape show similarity with the nervous impulse. Altering the environment (pH, Ca2+, temperature, etc.) changes the material properties of the membrane (e.g. lateral compressibility), and the observed pulse characteristics (velocity, amplitude, period, etc.) generally agree with those expected from the compressibility profile. Furthermore, these characteristics also appear consistent with pulses seen in various excitable systems (squid axons, algae, etc.) under varying environmental conditions (e.g. increase in conduction velocity with increase in temperature). These results altogether show that the signaling properties along the interface can be derived from its state diagram and the thermodynamic properties, and they support a physical basis of communication in living systems.

CPP 13.5 Mon 16:00 H10

Stochastic dynamics of nanoparticle and virus uptake — •Felix Frey, Falko Ziebert und Ulrich Schwarz — Institute for Theoretical Physics and BioQuant-Center, Heidelberg University, Germany

Biological cells constantly transport material and information across their plasma membrane. In particular cells routinely take up particles of diverse shapes and sizes between 10-300 nm, especially viruses, which often come in either spherical or cylindrical shapes. In general, particle uptake requires that the gain in adhesion energy overcomes the cost of plasma membrane bending. We first show by using a simple deterministic model that cylindrical particles are taken up faster than spherical particles for the same radius and volume. We then investigate stochastic effects, which might be relevant because of the small system size. We find that now spherical particles can be taken up faster because the mean first passage time is affected by multiplicative noise for the sphere rather than additive noise as in the case of the cylinder. Our findings suggest that stochasticity is equally important as geometry during particle uptake.

CPP 14: Organic photovoltaics and electronics (joint session HL/CPP)

Time: Monday 15:00–17:15 Location: H31

CPP 14.1 Mon 15:00 H31

Spectroscopy of Oligoacene molecules attached to Argon clusters — •Matthias Bohlen[1], Corey A. Rice[1], Aaron LaForge[1,2], and Frank Stienkemeier[1] — [1]Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg — [2]University of Connecticut, Department of Physics, 2152 Hillside Rd, Storrs, CT, USA

Energy conversion efficiency for solar cells is generally limited by the Shockley-Queisser limit [1]. One way to circumvent this limit is through the use of organic photovoltaics (OPV), where specific charge and energy transfer processes can lead to higher conversion efficiencies. Polyaromatic hydrocarbons such as oligoacene molecules exhibit interesting quantum effects such as singlet fission, triplet-triplet annihilation, or superradiance and make promising candidates for OPV applications. Recently anthracene, tetracene and pentacene molecules adhered to the surface of neon clusters have been shown to provide interesting model systems for detailed studies of such effects [2]. We want to extend these measurements by spectroscopy of oligoacenes deposited to the surface of argon clusters.

[1] W. Shockley and H. J. Queisser, J Appl Phys 32, 510 (1961)

[2] S. Izadnia et al., J. Phys. Chem. Lett.*8,*2068 (2017)

CPP 14.2 Mon 15:15 H31

When the model description hampers the parameter extraction for organic thin-film transistors — Markus Krammer[1], James Borchert[2], Andreas Petritz[3], Gerburg Schider[3], Esther Karner-Petritz[3], Barbara Stadlober[3], Hagen Klauk[2], and •Karin Zojer[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz, Austria — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Joanneum Research Materials, Weiz, Austria

When transistor parameters, like charge mobility or contact resistances, are determined from the electrical characteristics, their values are not unambiguous, but rather depend on the extraction technique and on the underlying transistor model. We propose a technique to establish whether the ambiguity arises already from the chosen transistor model. This two-step technique analyzes the electrical measurements of a series of TFTs with different channel lengths. The first step extracts the parameters for each individual transistor. The second step checks whether the channel length-dependence of the extracted parameters is consistent with the model. We demonstrate the technique for a range of organic TFTs that differ in the semiconductor, the injecting contacts, and the geometry. Independent of the transistor set, state-of-the-art transistor models fail to reproduce the correct channel length-dependence. Our technique suggests that transistor models require improvements in terms of carrier density dependence of the mobility and the consideration of uncompensated charges in the transistor channel.

CPP 14.3 Mon 15:30 H31

Vibronic coupling governs ultrafast intermolecular energy transfer in an oligomer thin film — Ephraim Sommer[1], Xuan Trung Nguyen[1], Lynn Gross[2], Thomas Frauenheim[2], Elena Mena-Osteritz[3], Peter Bäuerle[3], •Antonietta De Sio[1], and Christoph Lienau[1] — [1]Institut für Physik, Universität Oldenburg — [2]BCCMS, Universität Bremen — [3]Institut für organische Chemie II und neue Materialien, Universität Ulm

Organic photovoltaic(OPV) materials are complex molecular systems with many vibrational degrees of freedom. In such large molecules, vibronic coupling may result in conical intersections(CIs) of potential energy surfaces. Close to CIs, large vibronic couplings induce efficient ultrafast transition between electronic states. Hence CIs may profoundly influence the dynamics and yield of energy and charge transfer processes. So far, however, the importance of CIs for OPV materials has not yet been discussed. Here we use ultrafast two-dimensional electronic spectroscopy to study the light-induced dynamics in an oligomer thin film for OPV. Upon impulsive excitation, we detect a grid-like peak pattern suggesting coherent wavepacket motion in the excited state. After <50fs, the pattern transforms into a broad, featureless single peak. We observe an increase of oscillation period with an abrupt vanishing of the optically excited wavepacket, followed by the emergence of a new wavepacket with different oscillation. These results, together with ab-initio molecular dynamics calculations, show that intermolecular energy transfer in stacked dimers of this oligomer involves passage of the optically excited wavepacket through a CI within <50fs.

CPP 14.4 Mon 15:45 H31

Influence of thermal transport parameters on operation temperature of OLEDs — •Georgii Krikun and Karin Zojer — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz, Austria

Utilizing organic light emitting diodes (OLEDs) for lighting requires a homogeneous operation across large surface areas. This poses the challenge to suppress local variations in temperature and current density. While OLED research mostly focuses on electric and optical properties, thermal properties are highly relevant, as charge transport in organics is thermally activated. Due to the peculiar coupling between thermal and charge transport, related properties cannot be decoupled from each other.

We investigate how thermal conductivity and heat transfer between OLED surface and environment impact current voltage relations and device temperature for a given ambient temperature. By using self-consistent drift-diffusion based simulations, that simultaneously account for thermal and charge transport and their coupling, we establish how excess heating can be effectively counteracted. Despite a strong coupling between charge and heat transport, heat transport is essentially governed by layers that not participate in charge transport. Hence, electrical and thermal properties can be tuned with separate layers.

15 min. break

CPP 14.5 Mon 16:15 H31

Barrier Heights in Contacts to Electroluminescent Thin Films of 1-(pyridin-2-yl)-3-(quinolin-2-yl)imidazo[1,5-a]quinoline Determined by Kelvin Probe Force Microscopy — •Clemens Geis[1], Georg Albrecht[1], Julia Ruhl[2], Jasmin Martha Herr[2], Richard Göttlich[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik — [2]Justus-Liebig-Universität Gießen, Institut für Organische Chemie

Thin films of 1-(pyridin-2-yl)-3-(quinolin-2-yl)imidazo[1,5-a]quinoline ($PCIC$) were prepared by physical vapor deposition and analyzed in situ by Kelvin probe force microscopy (KPFM). As contact phases, poly(3,4-ethylenedioxythiophene) polystyrene sulfonate ($PEDOT : PSS$) and poly(9-vinylcarbazole) (PVK) were used as hole conductors and bathocuproine (BCP) as electron conductor. Charge carrier injection barriers were identified, electroluminescent layer structures were prepared and effects of contact formation on radiative recombination were studied. Aside from the expected blue emission, a significantly red-shifted emission was found and assigned to electroplex formation with BCP. Using $PCIC$ in a host-guest system within a matrix of PVK led to blue emission at improved luminescence. The studied interactions of $PCIC$ with typical contact materials reveal the potential and limitations of $PCIC$ as an electroluminescent material.

CPP 14.6 Mon 16:30 H31

Rubrene based diodes for rectification applications — •Michael Sawatzki[1], Bahman Kheradmand Boroujeni[2], Hans Klemann[1], Frank Ellinger[2], and Karl Leo[1,3] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, 01187 Dresden, Germany — [2]Chair for Circuit Design and Network Theory (CCN), Technische Universität Dresden, 01069 Dresden, Germany — [3]Center for Advancing Electronics Dresden (cfaed), 01187 Dresden, Germany

The developement of organic electronics is usually focused on a small set of electronic components, mainly OLEDs, solar cells, and various types of OFETs. To realize circuits, additional devices are required. One such device type are high-speed diodes, in the role of rectifiers, voltage stabilizers or analog signal processing. In particular for high-frequency RFID-applications it is essential to provide fast-switching diodes. The performance of such devices is closely related to the mobility of the semiconductor materials in use. Due to the anisotropy of charge carrier transport in most high-mobility organic semiconductors, it is necessary to find material systems that offer high vertical mobilities. We present organic diodes, optimized for transition-frequency and high driving current, utilizing highly crystalline layers of Rubrene. These diodes show record values for the transition frequency, both in open circuit and under load. The values rached are higher than for inorganic diodes based on amorphous silicon and therefore allow for a low-cost realization of medium to long range RFID-systems.

CPP 14.7 Mon 16:45 H31

Non-fullerene acceptors with tailored properties for organic solar cells — •Anastasia Markina[1], Frederic Laquai[2], and Denis Andrienko[1,2] — [1]Max Planck Institute for Polymer Research, Mainz 55128, Germany — [2]King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Thuwal 23955-6900, Kingdom of Saudi Arabia

One promising method to achieve higher solar cell efficiencies is to replace fullerenes with strongly-absorbing dye molecules, namely, non-fullerene acceptors (NFAs). However, the systematic design of acceptor molecules with tailored properties has yet to be demonstrated. The main difficulty here is that, while fullerenes are electrostatically inert, new acceptor molecules typically have strong static quadrupole moments.

By exploring the long-range electrostatic interaction at the interface, we demonstrate that, for a set of recently developed NFAs, the electrostatic bias potential can be directly related to the stabilization (or destabilization) of charge-transfer (CT) states as well as changes of the photovoltaic gap.

We find that the correlation between quadrupole moments, charge separation efficiency, and CT-state energy predicted by our model, is experimentally reproduced for several different donor /acceptor combinations. This allows us to predict new NFA structures using combinations of readily available molecular building blocks that can potentially reach even higher performances than those currently achieved in state-of-the-art NFA devices.

CPP 14.8 Mon 17:00 H31

The three optical signatures of p-doping in poly(3-hexylthiophene) — Malavika Arvind[1], •Claudia Tait[2], Jan Behrends[2], and Dieter Neher[1] — [1]Universität Potsdam, Potsdam, Germany — [2]Freie Universität Berlin, Berlin, Germany

Doping is an important process in the realization of electronic devices. Here we investigate the mechanism of p-doping of regioregular- and regiorandom- poly(3-hexylthiophene) (P3HT) using two dopants - F4TCNQ and tris(pentafluorophenyl)borane (BCF). Although both dopants exhibit Integer Charge Transfer (ICT) with rreP3HT in solution, the sub-band gap features in the UV-Vis-NIR spectra of F4TCNQ- and BCF-doped rraP3HT differ significantly.[1] The concentration and nature of paramagnetic states generated in the different systems was investigated using EPR spectroscopy. The results reveal significantly reduced spin concentrations in the doped rraP3HT solutions, in particular with F4TCNQ as dopant, supporting the existence of EPR-silent bound charge pairs. Additionally, the hole delocalization was shown to be reduced in regiorandom- compared to regioregular-P3HT. We conclude that CTC and ITC formation is not specific for thiophene-based polymers and oligomers, respectively, as suggested by earlier results. [2] Instead, the nature of the doping-induced state correlates strongly with the ability of the conjugated backbone to planarize and to delocalize the polaron along the conjugated system.

[1] Pingel P., Arvind M. et al. (2016). Adv. Electron. Mater.,2:1600204 [2] H. Méndez, I. Salzmann, et al., Nat. Commun. 6, 8560 (2015).

CPP 15: Symposium SYCO of the divisions MM (leading), O, CPP, KFM and DS continued as topical session: Mechanically controlled electrical conductivity of oxides (joint session MM/CPP/O)

Sessions: SYCO II and III

Time: Monday 15:45–18:30 Location: H46

Topical Talk CPP 15.1 Mon 15:45 H46

Probing the properties of dislocations in SrTiO$_3$ through transient transport measurements — •Roger De Souza — Institute of Physical Chemistry, RWTH Aachen University, 52056 Aachen, Germany

There is renewed interest in the interaction between oxygen vacancies and dislocations in the perovskite oxide SrTiO$_3$, driven by the material's possible application in devices for all-oxide electronics and for resistive switching. In my talk, I will demonstrate how transient transport experiments — comprising ^{18}O/^{16}O isotope exchanges and Secondary Ion Mass Spectrometry (SIMS) analysis — can be used to obtain a deeper understanding of this interaction. Having first introduced the thermodynamics of space-charge formation at extended defects, I will focus on describing experiments and simulations on various geometries: annealed single crystals, bicrystals, and polished single crystals. Finally, I will discuss how these studies allow us to arrive at a consistent description of point-defect behaviour at dislocations in SrTiO$_3$.

CPP 15.2 Mon 16:15 H46

Characterization of Fe:STO thin films prepared by pulsed laser deposition — •Maximilian Morgenbesser, Stefanie Taibl, Markus Kubicek, Alexander Viernstein, Christopher Herzig, Andreas Limbeck, and Jürgen Fleig — TU Wien, Wien, Österreich

The perovskite-type oxide SrTiO3 (STO) is one of the best investigated materials in solid state ionics and commonly used as a model material in solid state ionics. The defect model of bulk SrTiO3 is well understood and the conductivity of bulk samples can be tailored by acceptor or donor doping, e.g. with Fe3+ or Nb5+ on the Ti4+ site. However, other aspects of SrTiO3 have not been understood so far, for example the the influence of factors such as stoichiometry and strain on the conductivity which is investigated in this study.

Two different kinds of 2 % Fe-doped thin films were deposited by pulsed laser deposition (PLD). Thin films deposited from stoichiometric targets exhibit a low, intrinsic conductivity. In addition, targets with Sr overstoichiometry were used and the conductivity could be increased by four orders of magnitude. The thin films are compared to each other in regard to the structure and stoichiometry. Structural differences could be found by x-ray diffraction measures, revealing a difference in lattice parameters. The chemical composition was analyzed by means of inductively coupled plasma optical emission spectroscopy (ICP-OES) and differences in the A/B ratios could be found. A model linking the conductivity to the stoichiometry of the thin films is presented, highlighting the possible impact of cation vacancies and antisite defects on the electrical conductivity of Fe:SrTiO3.

CPP 15.3 Mon 16:30 H46

Generation of controlled dislocation structures in SrTiO3 and TiO2 for elucidating dislocation impact on electrical properties. — •Lukas Porz, Till Frömling, and Jürgen Rödel — Institute of Materials Science, Technische Universität Darmstadt, 64287 Darmstadt, Germany

Dislocations have been understood to alter numerous functional properties of ceramic materials, such as conductivity[Whitworth 1975]. Recently, modification of functional properties of oxide materials by dislocations receives much attention due to their various potentials for application[Szot 2018]. Especially the complex dislocation structure of naturally occurring dislocations makes investigations of dislocation effects difficult. Thus, disentangling the different effects of dislocations requires an ordered structure of the dislocations. So far ordered structures were primarily fabricated in bi-crystal interfaces which are often not comparable to natural dislocation arrangements.

We present a route to control the arrangement of the dislocations locally. Different slip systems can be individually introduced and an arrangement of all dislocations lying in the same set of slip planes was achieved. With identical line vectors, the dislocations connect two surfaces of a bulk sample which was shown by dark field x-ray microscopy.

This well-arranged and well-understood structure of dislocations is a pre-requisite for unambiguous interpretations of detailed experiments on functional properties. The value of a controlled arrangement of dislocations is demonstrated by conductivity data along dislocation lines and across slip bands in comparison to a dislocation free reference.

45 min. break

CPP 15.4 Mon 17:30 H46

Atomic and electronic structure of wurtzite ZnO(0001) inversion domain boundaries — •Jochen Rohrer and Karsten Albe — FG Materialmodellierung, FB Material- und Geowissenschaften, Technische Universität Darmstadt

In a recent work [1], variations of the conductivity of ZnO bicrystal samples with (0001)||(0001) and $(000\bar{1})|(000\bar{1})$ orientations (inversion domain boundaries, IDB) due to the modulation of the potential barrier height at the IDB with respect to strain [2] has been demonstrated. In order to establish a more profound understanding of this behavior, a detailed characterization of the atomic structure and electronic properties of such IDBs by means of first-principles methods will be valuable. However, despite the structural and chemical variability of this system, only a few atomistic models have been in studied to date [3].

In this work we comprehensively study ZnO{0001} IDBs by means of density functional theory calculations. In particular, we construct a variety of structurally and chemically different phase-pure models and identify their thermodynamic stability within the allowed range of the O chemical potential. For stable models we investigate electronic properties and their response to strain. Finally we also study the role of various dopants, commonly added in experimental bicrystal samples.

[1] P. Keil *et al.*, *Adv. Mater.* **30**, 1705573 (2018). [2] D. R. Clarke, *J. Am. Ceram. Soc.* **82**, 485 (1999). [3] S. Li *et al.*, *Phys. Status Solidi B* **255**, 1700429 (2017).

CPP 15.5 Mon 17:45 H46

Impact of internal electric field on the grain boundary barrier height of ZnO — •Bai-Xiang Xu, Ziqi Zhou, and Till Frömling — Institute of Materials Science, TU Darmstadt

Polycrystalline ZnO ceramics with grain boundary potential barriers are important materials for surge arresters due to their non-linear current-voltage behavior, and have potential application in advanced devices. Different grain boundary barrier height models have been developed by considering the direct piezoelectric effect. However, the piezoelectric charge should not only result from the direct piezoelectric effect, but also from the inverse piezoelectric effect, which refers to the mechanical response of the material by the electric field. Due to the charges at the grain boundary, strong internal electric field can be expected, and it leads to strain change through the inverse piezoelectric effect. This strain further modifies the polarization and thus leads to additional piezoelectric charges at the grain boundary and in the depletion layer. Thus, this should also be taken into account self-consistently. For this purpose we employ both analytical model and finite-element numerical simulation to reveal the impact of internal electric field on the GB barrier height and its stress sensitivity. Results show that the piezoelectric charge induced by the internal field tends to adjust the grain boundary charge and lowers the barrier height. Furthermore, the barrier height becomes less sensitive to mechanical stress and applied voltage if the influence of the internal field is taken into account. The extended model with the inverse piezoelectric effect of the internal field allows to further elucidate their piezotronic response.

CPP 15.6 Mon 18:00 H46

Influence of cation order and strain on Na diffusion in $Na_3Zr_2Si_2PO_{12}$: A computational study — •Lisette Haarmann and Karsten Albe — Technische Universität Darmstadt, Otto-Berndt-Str. 3 64287 Darmstadt

$Na_3Zr_2Si_2PO_{12}$ is a solid electrolyte which is part of the Na super ionic conductor (NASICON) family. Experimentally, only Si/P lattice positions can be determined, but not the distribution of P on these sites[1]. This distribution, however, plays a crucial role for the Na diffusion. A systematic study of different cation orders is conducted using Molecular Dynamics (MD) simulations. Due to the strong correlation of diffusion in this material, the calculation of D_σ is necessary to obtain the ionic conductivity from the Nernst-Einstein equation[2]. By calculating D_σ and the tracer diffusion coefficient D_{tr}, Haven ratios are determined. Additionally, a jump rate model was developed, which allows investigation of correlation between individual jumps.

Moreover, it has been reported that doping can strongly increase the diffusivity of Na in NASICON materials[3]. In many cases, this is attributed to enlarged bottlenecks of diffusion. These doping elements, however, do not only contract or dilate the lattice structure but alter the chemical environment of the Na ions as well. In an effort to study purely the effect of mechanical deformation, the strain dependence of D_{tr} and the activation energy E_A is investigated.

[1] Boilot, J.P., *et. al.*, Journal of Solid State Chemistry **73**, (1988)
[2] Murch, G., Solid State Ionics **7**, (1982)
[3] Guin, M., Tietz, F., Journal of Power Sources **273**, (2015)

CPP 15.7 Mon 18:15 H46

The impact of mechanical stresses on the ionic conductivity of nanoparticles — •Peter Stein[1], Bai-Xiang Xu[1], and Karsten Albe[2] — [1]TU Darmstadt, FB 11, FG Mechanik funktionaler Materialien — [2]TU Darmstadt, FB 11, FG Materialmodellierung

Nanostructured electrodes have found wide application in electrochemical systems, for instance for lithium-ion batteries. This is due to their featuring short diffusion paths and large surface areas, allowing for comparatively fast surface reactions and transport within the slender bulk material. At this length-scale, surface stresses acting on the electrode surface induce a (non-uniform) pressure within the material, providing mechanical stabilization. As a result, nanostructured electrodes exhibit high reversible capacities and stable cycling behavior [1] as well as a higher robustness against mechanical degradation [2]. However, the surface-induced pressure field also affects the electrochemical behavior of the particle, modifying, among other things, surface reaction rates and ionic mobility.

In this contribution, we discuss the interaction of mechanical stresses with the electrochemical behavior of nanostructured electrode particles. We thereby consider ideal analytical shapes, faceted nanoparticles, and regular nanostructures such as inverse opal electrodes. We further demonstrate the impact of surface-stress-induced mechanical fields on defect thermodynamics and kinetics, chemical reactions, and phase transformations.

[1] N. Zhao et al., Pure Appl. Chem. 80:2283-2295, 2008. [2] C.K. Chan et al., Nat. Nanotechnol. 3:31-35, 2008.

CPP 16: Glasses and Glass Transition (joint session CPP/DY)

Time: Monday 16:15–17:30 Location: H8

CPP 16.1 Mon 16:15 H8

A coarse-grained model for studying polymer melts toward the glass transition point under cooling — •Hsiao-Ping Hsu and Kurt Kremer — Max Planck Institute for Polymer Research, Mainz, Germany

For studying polymer melts of weakly semiflexible chains under cooling at zero pressure by molecular dynamics simulations, a coarse-grained model based on the standard bead-spring model is developed. We introduce a short range attractive potential between non-bonded monomers such that the pressure of polymer melts is tuned to zero. Additionally, the common used bond-bending potential [Everaers et al., Science 303, 823 (2004)] controlling the chain stiffness is replaced by another new bond-bending potential. With our newly developed model, we show that the Kuhn length and the internal distance of chains in a melt are independent of temperatures under cooling. The glass transition is probed by the volume change of polymer melts and the slowing down of the mobility of chains. Thus, our coarse-grained model can be served as an optimal model for studying glass-forming polymer melts and understanding the effect of free surface on the glass transition of thin polymer films.

CPP 16.2 Mon 16:30 H8

Molecular Dynamics of Dipole Functionalized Triphenylene-based Discotics — •Arda Yildirim[1], Andrea Bühlmeyer[2], Shunsuke Hayashi[3], Johannes Christian Haenle[2], Kathrin Sentker[4], Patrick Huber[4], Sabine Laschat[2], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und *prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany — [2]Institut für Organische Chemie, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany — [3]Department of Applied Chemistry, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan — [4]Materials Physics and Technology, Hamburg University of Technology (TUHH), 21073 Hamburg, Germany

In this study, the molecular dynamics of a series of dipole functionalized triphenylene-based discotics, forming a columnar mesophase, were investigated by broadband dielectric spectroscopy (BDS). In addition to conductivity and localized dynamics, glassy dynamics were also observed. At higher temperatures an $\alpha 1$-processes and at low temperatures an $\alpha 2$ processes were detected having a completely different temperature dependence of its relaxation times. Different molecular assignments of $\alpha 1$- and $\alpha 2$-processes are suggested. The phase behavior of the material was explored under helium purge down to 100 K by differential scanning calorimetry (DSC). Besides the phase transition temperatures and enthalpies, one or two thermal glass transitions were found for all the materials. Moreover, the glassy dynamics were further investigated by Flash DSC, which is a chip-based calorimetry technique allowing for fast heating and cooling rates as high as 10000K

CPP 16.3 Mon 16:45 H8

System size-dependent non-affine displacements in a model glass: the impact of yield strain — •Moumita Maiti and Andreas Heuer — University of Muenster, Institute for physical chemistry, Corrensstr. 28/30, 48149, Muenster

The probability distribution of non-affine displacements has an exponential tail, which is scaled with the system size. The scaling exponent is zero for all strains below a critical value which turns out surprisingly to be the overshoot strain. Above, the scaling exponent is finite. This picture holds for the system size larger than approx. 4000 particles. For small system size we find that the scaling exponent is finite and constant irrespective of any strain value. In order to understand these two pictures we calculate the mobility correlation of nearest neighbours. Around the mobility range where percolation of mobile particles takes place, the correlation increases again up to sizes of approx. 4000 particles and saturates above that size. This yields additional insight into the physical mechanisms of yielding.

CPP 16.4 Mon 17:00 H8

Tuning the Temperature-Dependent Thermal Conductivity via Complex Colloidal Superstructures — Fabian Nutz and •Markus Retsch — Physical Chemistry I, University of Bayreuth, 95447 Bayreuth, Germany

The ability to specifically tune the temperature dependence of the thermal conductivity possess a vital challenge to develop and conceive future heat management devices. In this contribution, we demonstrate the vast potential of polymer colloidal crystals to address and master these challenges. We achieve this goal based on the constriction controlled thermal transport through well-defined colloidal crystal superstructures.[1,2,3,4] These colloidal superstructures are specifically built by tailor-made latex particles with distinct glass transition temperatures. We exploit their multiresponsive film formation at various temperatures to demonstrate unprecedented control over thermal conductivity at temperatures between 25 °C and 200 °C. Based on the film formation process, we can irreversibly increase the thermal conductivity by a factor of about three. We show how to control: i) the temperature, where the increase in thermal conductivity happens ii) the sharpness of the thermal conductivity increase iii) the height of the increase in thermal conductivity iv) the incorporation of a multistep increase in thermal conductivity

[1] Nutz et al. J. Colloid Interface Sci. 2015, 457, 96. [2] Ruckdeschel et al, Nanoscale 2015, 7, 10059. [3] Nutz et al, Phys. Chem. Chem. Phys. 2017, 19, 16124

CPP 16.5 Mon 17:15 H8

Direct Determination of the Thermodynamic Properties of Melting for Amino Acids — •Y.Z. Chua[1], H.T. Do[3], D. Zaitsau[2], S.P. Verevkin[2], C. Held[3], and C. Schick[1] — [1]Uni. Rostock, Inst. Physics and CALOR, Rostock, Germany — [2]Uni. Rostock, Inst. Chemistry, Rostock, Germany — [3]TU Dortmund Uni., Depart. Biochem. Chem. Eng., Dortmund, Germany

The properties of melting are used for the prediction of solubility of solid compounds. Unfortunately, by using the conventional DSC or adiabatic calorimetry direct determination of the melting enthalpy and melting temperature 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 $2\cdot 10^4\ K\cdot s^{-1}$ are utilized with fast-scanning calorimeter Mettler Toledo Flash DSC1, which employs thin film chip sensors with sub $\mu J\cdot K^{-1}$ addenda heat capacities. With the help of this technique the melting parameters for a series of amino acids and dipeptides 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. The determined glass transition temperatures agree with the Beaman-Kauzmann rule. The correlation between the melting properties of the amino acids and dipeptides with their molecular structures were investigated.

CPP 17: Poster Session I

Topics: Active Matter (17.1-17.3); Biopolymers, Biomaterials and Bioinspired Functional Materials (17.4-17.8); Charged Soft Matter, Polyelectrolytes and Ionic Liquids (17.9-17.17); Crystallization, Nucleation and Self-Assembly (17.18-17.22); Electrical, Dielectrical and Optical Properties of Thin Films (17.23-17.25); Glasses and Glass Transition (17.26-17.32); Interfaces and Thin Films (17.33-17.39); Physics of Self-Organization in DNA Nanostructures (17.40-17.42); Polymer Networks and Elastomers (17.43-17.44).

Time: Monday 17:30–19:30 Location: Poster B1

CPP 17.1 Mon 17:30 Poster B1

Translocation in Presence of Molecular Motors — •Iman Abdoli, Hidde Vuijk, and Abhinav Sharma — Leibniz Institute for Polymer Reseach

We study the assisted translocation of a polymer chain across a membrane nano-pore, on one side of which there are molecular motors. These motors can attach from the bulk on to the polymer, perform directed motion on the chain, and can undergo detachment. We model the directed motion of the motors using the Totally Asymmetric Random Process (TASEP) and the attachment/detachment using Langmuir Kinetics (LK). We study, analytically and computationally, how motors influence the rate of translocation of polymer chain across the membrane.

CPP 17.2 Mon 17:30 Poster B1

Fabrication of ellipsoidal microswimmers with controllable tip shape — •Yara Alsaadawi[1], Fernando Vazquez Luna[2], Anna Eichler-Volf[1], Martin Steinhart[2], and Artur Erbe[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Institute of Chemistry of New Materials and Center of Physics and Chemistry of New Materials, Universität Osnabrück, 49076 Osnabrück, Germany

Microswimmers are objects capable of converting applied energy into active motion, resulting in its propulsion in a medium. The shape and chemical compound of the microswimmer strongly influence its propulsion properties. Here we investigate a template-based approach for fabrication of particles with controlled composition, size, and shape, which can be used as fundamental units for the preparation of microswimmers. Polystyrene nanorods with different configurations of the tip shape were fabricated with an aspect ratio of 10:1. The ratio of length-to-width (i.e. aspect ratio) can be easily modified by controlling the surface properties of the template. The wettability transition of polystyrene was used to manipulate the morphology and entrapment of polymer nanostructures.

CPP 17.3 Mon 17:30 Poster B1

Modeling the interaction of magnetically capped colloidal particles — •Maximilian Neumann[1], Sibylle Gemming[1,2], Gabi Steinbach[2], and Artur Erbe[1] — [1]Institute of Physics, TU Chemnitz, D-09107 Chemnitz — [2]Helmholtz-Zentrum Dresden - Rossendort, D-01328 Dresden

Colloidal self-assembly bears significant potential for the bottom-up fabrication of advanced materials and micromechanical structures. A wide range of particles with different types of anisotropy have been recognized as promising precursors for controlled structure engineering. Here, we concentrate on particles that interact via polar fields, which are intrinsically anisotropic. More specifically, we focus on the assembly of micron-sized silica spheres which are partly covered by a thin ferromagnetic layer with an out-of-plane magnetic anisotropy. To study assemblies of such magnetic particles, we introduce a simple two-parameter model: The extended magnetization distribution is approximated by a current-carrying coil enclosed inside a hard sphere. The far field of that current reproduces the stray field of a point dipole model, the near field reflects an extended magnetization. Such a model employs only two parameters to describe the shape of the magnetization distribution: The radius and the position of the coil inside the sphere. We present stable assemblies as a function of both parameters. In the limit of very small coils the analytical solution for two particles with shifted point dipoles is correctly reproduced. By increasing the radius of the coil, we reproduce experimentally observed particle arrangements not covered by models based on single shifted dipoles.

CPP 17.4 Mon 17:30 Poster B1

Biopolymer templated titanium dioxide films prepared via spray coating — •Julian Heger[1], Wei Chen[1], Sebastian Grott[1], Xinyu Jiang[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS für Funktionelle Materialien, 85748 Garching, Germany — [2]Elettra-Sincrotrone Trieste S.C.p.A., Trieste, Italy

Nanostructured titanium dioxide films have great potential for application in photovoltaics, such as the inorganic counterpart in hybrid solar cells. For this purpose, the film morphology has crucial influence on the device performance, since a high surface-to-volume ratio is needed for efficient charge separation. So far, inorganic mesoporous matrices are successfully achieved by sol-gel chemistry in combination with block copolymer directed templating. As a novel approach, we use environmentally friendly biopolymers as tailoring agents. The whey protein ß-Lactoglobulin was found to form different structures within denaturation, from fibrils to spheres. By combining heat denaturation at different pH and sol-gel chemistry, different nanosized structures are introduced into titanium dioxide. The resulting sol-gels are used as inks for film deposition via spray coating. After calcination to remove the biopolymer template, the film morphologies of the remaining titanium dioxide scaffolds are investigated by grazing incidence small-angle X-ray scattering (GISAXS). GISAXS measurements are supplemented by scanning electron microscopy.

CPP 17.5 Mon 17:30 Poster B1

Water-Mediated Protein-Protein Interactions at High Pressures are Controlled by a Deep-Sea Osmolyte — Karin Julius[1], Jonathan Weine[1], Nico König[1], Mimi Gao[2], Jan Latarius[1], •Michael Paulus[1], Martin A. Schroer[3], Metin Tolan[1], and Roland Winter[2] — [1]Faculty of Physics/DELTA, TU Dortmund University, 44221 Dortmund, Germany — [2]Faculty of Chemistry and Chemical Biology, TU Dortmund University, Otto-Hahn-Strasse 4a, 44227 Dortmund, Germany — [3]European Molecular Biology Laboratory (EMBL) Hamburg c/o DESY, Notkestrasse 85, 22607 Hamburg, Germany

Living cells accumulate organic osmolytes to high concentrations as adaptive response towards external stressors such as dehydration, freezing, salinity or high hydrostatic pressure as encountered in the deep sea. The mechanisms of protein stabilization and the linkage to the intermolecular interactions between proteins in the cellular milieu at ambient as well as at elevated pressures are still largely terra incognita. Herein, we study the impact of natural osmolyte mixtures on the pressure dependent intermolecular pair-interaction potential of dense protein solutions by applying small-angle X-ray scattering in combination with a liquid-state theoretical approach. Particularly, the presence of the deep-sea osmolyte TMAO guarantees the sustainability of the native protein fold under harsh environmental conditions. Further, we find a strong interplay between water and osmolyte in controlling the water-mediated intermolecular interactions at high pressure, thereby preventing contact formation and hence aggregation of proteins.

CPP 17.6 Mon 17:30 Poster B1

Towards biomimetic carbon nanomembranes — •Raphael Dalpke[1], Anna Dreyer[2], Thorsten Seidel[2], André Beyer[1], Karl-Josef Dietz[2], and Armin Gölzhäuser[1] — [1]Physics of Supramolecular Systems and Surfaces, Faculty of Physics, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany. — [2]Biochemistry and Physiology of Plants, Faculty of Biology, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany.

Cell membranes are a prerequisite for life. Incorporated membrane proteins facilitate the transfer of substances. To explore the mechanisms of vectorial transport across cell membranes, an ultrathin, biomimetic system is desirable which allows the controlled integration of proteins. Here, we present different strategies to immobilize proteins with high affinity on carbon nanomembranes (CNMs). Covalently bonded aromatic precursor molecules form self-assembled monolayers (SAMs) on metal surfaces. After the irradiation with low energy electrons (100 eV) these cross-link to mechanically stable, chemically inert, and permeable CNMs with a typical thickness of around 1 nm which can be transferred onto any arbitrary substrate for further usage [1]. In particular, we discuss functionalization strategies for reversible as well as for irreversible protein immobilization. The basis of the reversible type is the non-covalent interaction of streptavidin and biotin which can be released by d-desthiobiotin. The irreversible type is based on the maleimide coupling chemistry, where a stable thioether bond is formed.

[1] A. Turchanin and A. Gölzhäuser, Carbon Nanomembranes, Advanced Materials, 2016, 28 (29), pp. 6075-6103.

CPP 17.7 Mon 17:30 Poster B1

Biomimetical Surfaces for Pollutant Separation — •Sebastian Stelzner[1], Dagmar Voigt[2], Bernhard Alexander Glatz[1], and Andreas Fery[1] — [1]Leibniz-Institut für Polymerforschung, Dresden, Germany — [2]Institut für Botanik, Technische Universität Dresden, Germany

The cuticula is a main part of the evolutionary progress of terrestrial plants. It consists of an insoluble polymer fraction and a soluble lipid (wax). Those waxes are crystalloid micro- and nanostructures with a high structural and morphological diversity and can rearrange in a self-organized manner. The platelets, tubules, filaments etc. are forming based on their chemical composition and share the ability to regenerate. In order to utilize those properties, structured polymer substrates are produced with the target of adhesion and recrystallization of vaporized plant waxes. By tuning the chemical properties of the waxes as well as the surficial ones of the substrates, the shape and orientation of the crystals can be manipulated to the intended usage. In this project, environmental pollutant adhesion is targeted. The influence of surface-structured polymers on the wax crystallization is compared to flat substrates and the difference in grade of adhesion is analyzed and quantified. The aim is to generate an optimized material adhesion system. By separation and regeneration of the waxes or by the use of embedded catalysts, harmful air contaminants are sought to be decimated.

CPP 17.8 Mon 17:30 Poster B1

Secondary structure analysis of xanthan using atomic force microscopy — •Jenny Fjodorova[1], Julia Voss[2], Gerd Hublik[3], Vera Ortseifen[2], Karsten Niehaus[2], Volker Walhorn[1], and Dario Anselmetti[1] — [1]Experimental Biophysics and Applied Nanoscience, Bielefeld University, Germany — [2]Proteome and Metabolome Research, Bielefeld University, Germany — [3]Jungbunzlauer Austria AG, Pernhofen 1, 2064 Wulzeshofen, Austria

Xanthan is an extracellular polysaccharide, secreted by the bacterium *Xanthomonas campestris*. Due to its unique viscosifying properties over a wide range of salt concentrations, xanthan has numerous industrial applications e.g. in food, cosmetic or oil industry. Therefore, the optimisation of xanthan production and its rheological properties is of particular interest. Targeted genetic modification of the *Xanthomonas* metabolism and subsequent change of salt concentrations can be a powerful tool to optimise the shear-thickening potency and to improve the xanthan production efficiency.

Using atomic force microscopy (AFM) imaging and single molecule force spectroscopy (SMFS), we analysed the structure and the elastic characteristics of single xanthan polymers, which were produced by different *Xanthomonas* strains. We identified structures ranging from single-stranded coiled networks to branched double-strands. Taking into account the varying ability to form double-strands and differences in the bending stiffness, we observed a correlation between the formation of secondary structures and its resulting different viscosifying properties.

CPP 17.9 Mon 17:30 Poster B1

Structure of Ionic Liquid Mesophases inside Nanopore Confinement — •Andre Ultes[1], Julian Mars[1,2], Kathrin Sentker[3], Milena Lippmann[4], Forian Bertram[4], Patrick Huber[3], and Markus Mezger[1,2] — [1]Max Planck Institute for Polymer Research, Mainz — [2]Institute of Physics, Johannes Gutenberg University Mainz — [3]Institute of Materials Physics and Technology, Hamburg University of Technology — [4]DESY Photon Science, Hamburg

Ionic liquids composed of cations with long aliphatic side chains exhibit so-called microphase separation leading to structural heterogeneities on the nanometer length scale. Depending on their molecular structure, short range order as well as thermodynamically metastable and stable liquid crystalline (LC) mesophases have been observed [1]. Interfaces can strongly affect their phase stability and relative orientation [2]. In this work, the orientation and phase behavior of $[C_{22}C_1\mathrm{im}]^+[\mathrm{NTf}_2]^-$ inside anodized aluminum oxide (AAO) nanopores was investigated by X-ray scattering. Here, confinement can stabilize phases not observed in bulk. Depending on pore diameter and surface functionalization different orientations of the LC director relative to the pore axes were observed.

[1] H. Weiss et al., J. Phys. Chem. B, 121, 620 (2017).

[2] J. Mars et al., Phys. Chem. Chem. Phys., 19, 26651 (2017).

CPP 17.10 Mon 17:30 Poster B1

Influence of hydrocarbons on the bulk and surface structure of ionic liquids — •Julian Mars[1,2], Henning Weiss[1], Veijo Honkimäki[3], Bridget Murphy[4,5], Markus Bier[6,7], and Markus Mezger[1,2] — [1]Max Planck Institute for Polymer Research, Mainz — [2]Institute of Physics and MAINZ Graduate School, Johannes Gutenberg University Mainz — [3]ESRF The European Synchrotron, Grenoble — [4]Institute of Experimental and Applied Physics, Kiel University — [5]Ruprecht Haensel Laboratory, Kiel University — [6]Max Planck Institute for Intelligent Systems, Stuttgart — [7]University of Applied Sciences Würzburg-Schweinfurt

In supported ionic liquid (IL) phase catalysis, knowledge of the interfacial structure is essential to understand diffusion of reactants and products across IL/vapor interfaces. ILs composed of cations with long aliphatic side chains exhibit mesoscopic order and liquid crystalline mesophases. The solvate affinity to the ionic- and aliphatic domains of such ILs can strongly affect their structures adjacent to IL/vapor interfaces. We employ X-ray scattering techniques to investigate the bulk and near surface structure on the molecular length scale. For increasing alkane concentrations, we observe a shift of the first sharp diffraction peak to lower q-values. Originating from the mesoscopic order, this signature indicates aggregation of the non-polar alkanes in the aliphatic domains. Simultaneously, ionic liquid crystal transition temperatures decrease. At the surface, we observe the formation of adsorbate layers and surface induced smectic order.

CPP 17.11 Mon 17:30 Poster B1

Hydration forces on mica-electrolyte interfaces and their ion specificity — Simone van Lin[1], Igor Siretanu[1], •Kara K. Grotz[2], Nadine Schwierz[2], and Frieder Mugele[1] — [1]Physics of Complex Fluids Group and MESA+ Institute, Faculty of Science and Technology, University of Twente, Enschede, The Netherlands — [2]Department of Theoretical Biophysics, Max Planck Institute of Biophysics, Frankfurt am Main, Germany

Hydration forces play a fundamental role for a wide range of biological, chemical, and physical phenomena as they control the formation or prevention of direct contact between any kind of dissolved molecules or suspended particles in water. Here, we study the hydration of mica surfaces in contact with pure water as well as with aqueous alkali chloride salt solutions. Using molecular dynamics simulations in combination with atomic force micoscropy experiments, we demonstrate that hydration forces generally consist of both a monotonically decaying and an oscillatory part, each with unique dependence on the specific cation. In measurements, the monotonic hydration force gradually decreases in strength with decreasing ion size, leading to a transition from an overall repulsive (Li^+) to an overall attractive (Cs^+) total force. In simulations, the presence of strongly hydrated cations (Li^+) hardly disturbs the water structure, whereas weakly hydrated cations (Cs^+) suppress the pronounced layering of water at the interface, as well as the oscillatory part of the measured hydration force.

CPP 17.12 Mon 17:30 Poster B1

Correlated ion motion in lithium bis(trifluoromethanesulfonyl)imide – glyme solvate ionic liquids: Atomistic insights from molecular dynamics simulations — •Andreas Thum[1], Diddo Diddens[2], and Andreas Heuer[1] — [1]Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany — [2]Helmholtz-Institut Münster (IEK-12), Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany

Motional coupling of ions strongly influences the ionic conductivity of electrolyte solutions and ionic liquids (ILs). In both, the overall anticorrelated motion of like-charged ions reduces the conductivity compared to the ideal Nernst-Einstein conductivity. In electrolyte solutions, the overall correlated motion of opposite-charged ions lowers the conductivity, too. Contrary, in ILs this motional coupling is overall anticorrelated and enhances the conductivity.

To see how dynamic ion correlations evolve in time and space, we performed molecular dynamics simulations of mixtures of lithium bis(trifluoromethanesulfonyl)imide with glymes. These mixtures are known to form solvate ionic liquids (SILs) if mixed in a 1:1 molar ratio. The mixtures investigated here had molar ratios of 2:1, 3:2, 1:1, 1:2, 1:4 and 1:8, covering highly concentrated solutions, SILs and conventional solutions. We found that regarding the motional ion coupling the 2:1, 3:2, 1:1 and 1:2 mixtures behave like conventional ILs, whereas the 1:4 and 1:8 mixtures behave like conventional electrolyte solutions.

CPP 17.13 Mon 17:30 Poster B1

A mechanistic understanding of lithium ion transport in ternary electrolyte systems — •Alina Wettstein[1], Diddo Diddens[2], and Andreas Heuer[1,2] — [1]Institut für Physikalische Chemie, Corrensstraße 28-30, 48149 Münster, Germany — [2]Helmholtz-Institut Münster (HI MS), Corrensstraße 46, 48149 Münster, Germany

With regard to methodologically enhancing the electrolyte functionality, and hence the ionic conductivity as a crucial indicator, a profound understanding of the correlated ion motion is essential. For binary ionic liquid systems it has been shown that the motional coupling between ions is determined to a large extent by the conservation of momentum, concurring with simple theoretical relations for transference numbers that serve as a guideline for optimizing the electrolyte [1,2]. Inspired by this work, we perform Molecular Dynamics (MD) simulations to unravel the complex, and rather counterintuitive, interplay of dynamical electrostatic correlations in a ternary ionic liquid - lithium salt mixture, which contribute to the overall conductivity. From systematic analysis of a variety electrolyte compositions we try to identify key parameters that quantify the microscopic transport properties and serve as a constructive optimization concept.

[1] H. Kashyap et al., J. Phys. Chem. B, 2011, 115 (45), pp 13212-13221

[2] D. Diddens, V. Lesch and A. Heuer, Correlated Motion in Ionic Liquids. To be submitted., 2018

CPP 17.14 Mon 17:30 Poster B1

Foam film properties of NaPSS/C_{14}TAB-mixtures: Effect of added Salt — •Kevin Gräff, Larissa Braun, and Regine von Klitzing — Technische Universität Darmstadt, Soft Matter at Interfaces, Darmstadt, Germany

The properties of foams are of interest in many applications such as food technology, firefighting and in personal care products. To understand the properties of macroscopic foams it is important to investigate the single building blocks of it the so-called foam films, which separate the air bubbles from each other. Mixtures of oppositely charged polyelectrolytes and surfactants are widely used in industrial applications as they form highly surface active complexes. Many studies focus on different surfactant, different polyelectrolytes and their rations. However, the influence of the ionic strength - especially on the foam films - is still unclear. In this work, we use a thin film pressure balance (TFPB) to study the foam films of NaPSS/C_{14}TAB-mixtures in terms of the disjoining pressure inside the foam films, the surface potential at the air/water interface and the foam film stability. We add NaBr (the combination of the two counterions) to get insights on the effect of the ionic strength on the foam film properties.

CPP 17.15 Mon 17:30 Poster B1

Incorporating chemical reactivity into classical molecular dynamics simulations — •Myra Biedermann[1], Diddo Diddens[1,2], and Andreas Heuer[1,2] — [1]Institute of Physical Chemistry, University of Münster — [2]Helmholtz-Institut Münster

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 molecular dynamics (MD) simulations. Our methodological approach is inspired by work of Takenaka et al. [1]. There, reactive steps in form of Monte Carlo (MC) steps are introduced in addition to the standard MD steps in order to model chemical reactions within the system. Our specific realisation of those reactive steps differs from those in [1] inasmuch as it also uses information about the kinetics of the reactions (e.g. reaction rates) instead of only thermodynamic informations (e.g. reaction enthalpies). We use extensive ab initio molecular dynamics simulations to validate our approach as well as to estimate the required reaction rates which are used in the reactive molecular dynamics simulations.

This work is motivated by research on lithium ion batteries, more specifically by investigations regarding the molecular transport and reaction processes at the interface between electrode and electrolyte which lead to the initial formation of a Solid Electrolyte Interphase (SEI) and the formation of dendrites.

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

CPP 17.16 Mon 17:30 Poster B1

Protein condensation in the presence of lanthanide metal ions: relating local structure at the metal centres to phase behaviour — •Olga Matsarskaia[1], Sin-Yuen Chang[2], Felix Roosen-Runge[3], Stephen Parry[2], Giannantonio Cibin[2], Fajun Zhang[1], Sven L. M. Schroeder[4], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Diamond Light Source Ltd, Didcot, UK — [3]Lund University, Sweden — [4]University of Leeds, UK

Multivalent salts, e.g. YCl_3, have been shown to induce a liquid-liquid phase separation with a lower critical solution temperature (LCST-LLPS) in aqueous solutions of bovine serum albumin (BSA), providing an intriguing experimental framework for a comprehensive study of LLPS in proteins. Here, we attempt to connect the different levels of the description of LCST-LLPS from molecular-level to macroscopic. To this end, we examine the local chemical environment of the Y^{3+} cations using extended X-ray absorption fine-structure (EXAFS) spectroscopy. The EXAFS data show that the Y^{3+} coordination number (CN) decreases with increasing protein concentration and temperature due to the partial substitution of hydration water molecules around the Y^{3+} cations by protein carboxyl groups upon Y^{3+} coordination by the protein. The results of this study thus provide molecular-level evidence that hydration effects are key to LCST-LLPS in systems of BSA and multivalent salts.

CPP 17.17 Mon 17:30 Poster B1

Thermophoresis of a single colloidal particle — •Daniel Benjamin Mayer and Thomas Franosch — Institut für Theoretische Physik, Lepold-Franzens Universität, Technikerstraße 21A, A-6020 Innsbruck, Austria

We want to address the problem of a single charged colloid immersed in an electrolyte solution. In the presence of a temperature gradient, electrical body forces are no longer counter balanced by pressure gradients, thereby inducing solvent flow and a directed motion of the colloidal particle. In the limit of small temperature gradients, we numerically solve the associated field equations, including the non-linear Poisson-Boltzmann equation for the electrical potential and the steady Stokes equation governing the fluid flow.

The aim to calculate the thermal mobility is accompanied by difficulties since it appears as a boundary condition in the governing electrokinetic equations. However a decomposition of the problem into two auxiliary ones simplifies this task considerably. Furthermore we also examine the dependence of the thermal mobility on the surface potential and the Soret coefficient of the different ions in the electrolyte.

CPP 17.18 Mon 17:30 Poster B1

Nano-confinement on chain alignment and crystallization of conjugated polymers P3HT and PffBT4T-2OD by printed mesoporous TiO2 photoanodes — •Nian Li, Lin Song, Nitin Saxena, Wei Cao, Xinyu Jiang, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Control of n-type inorganic morphology, chain orientation and crystallization of the donor polymers is of significance in hybrid solar cells. Here, we use slot-die printing combined with wet chemistry to fabricate controllable mesoporous TiO2 nanostructures in large scale. Subsequently, the mesoporous TiO2 films with different pore size are backfilled with P3HT and PffBT4T-2OD, respectively, using two different ways of infiltration. TiO2 film morphology is investigated by scanning electron microscopy (SEM) and grazing incidence small-angle X-ray scattering (GISAXS). In order to investigate the effect of TiO2 pore size on the crystalline properties of the conjugated polymers P3HT and PffBT4T-2OD, e.g. lattice distance, crystal size or orientation, grazing incidence wide-angle X-ray scattering (GIWAXS) is applied to probe the hybrid films. Both P3HT and PffBT4T-2OD crystals with a denser packing of polymer chains exist in the large pore size of TiO2 films. For backfilling with PffBT4T-2OD, the face-on to edge-on ratio also prefers in the large-pore active layer.

CPP 17.19 Mon 17:30 Poster B1

Time-resolved X-ray scattering for the study of colloidal thin films — •Christopher Greve[1], Michael Buchhorn[1], Dinesh Kumar[2], Guillaume Freychet[2], Alexander Hexemer[2], Lutz Wiegart[3], and Eva M. Herzig[1] — [1]Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]ALS, Lawrence Berkley National Lab, 1 Cyclotron Road, Berkeley CA 94270, USA — [3]NSLSII, Brookhaven National Lab, Brookhaven Avenue, Upton NY, USA

X-Rays are a useful tool to investigate the dynamics and the morphology of hard and soft condensed matter. Synchrotron radiation makes it possible to probe short length scales ($<$ 100 nm) and long time scales ($>10^{-4}$ s). To obtain information about the underlying dynamics, during thin film formation, time-resolved measurements are investigated. We investigate slot-die coated thin films in situ in gracing incident geometry to gain insights into the underlying processes of thin film formation. For printing, an up-scalable printer setup is used and as a model system a drying colloidal suspension is examined. Such suspensions are widely used to investigate lattice growth, which is a technologically important research topic (e.g. programmable matter). As a model system, silica nanospheres are used. These feature under solvent evaporation a Kirkwood-Alder transition from amorphous to crystalline FCC thin films via an intermediate glass phase. In addition, a known Bain transition from FCC to BCC can take place under annealing. Using different experimental settings, we systematically study the effect of multiple scattering on the extracted dynamics of drying thin films to investigate the mentioned transitions.

CPP 17.20 Mon 17:30 Poster B1

Stabilization of tubular J-aggregates by silica coating for use in dry environment — •Katherine Herman, Holm Kirmse, Jürgen P. Rabe, and Stefan Kirstein — Humboldt Universität zu Berlin, Institut für Physik

The amphiphilic cyanine dye C8S3 is known to self-assemble in aqueous solution into tubular J-aggregates with a diameter of 13 nm and lengths exceeding microns. Their optical spectra are dominated by exciton bands which are very sensitive to structural changes. A major disadvantage of these aggregates is their low stability during drying. Here we use a coating of a thin layer of silica to stabilize these aggregates. In earlier work [1] shells of silica with controlled and homogeneous thickness of a few nanometer were synthesized around these aggregates without disrupting their optical spectra and hence their J-aggregate character. It is demonstrated here that these silica coatings mechanically and chemically stabilize the C8S3 J-aggregates and allow them to survive not only drying under ambient, but also under vacuum conditions of an electron microscope. Transmission electron microscope images confirm that the thickness of the silica coatings is 5 nm or less and energy dispersive X-ray spectroscopy confirms the presence of true silica. Emission spectra of dried silica coated samples indicate that the molecular structure of the aggregates is preserved and photobleaching under ambient conditions is significantly reduced.

[1] Y. Qiao, F. Polzer, H. Kirmse, S . Kirstein, and J.P. Rabe, Chem. Commun. 51, 11980 (2015)

CPP 17.21 Mon 17:30 Poster B1

Crystallization kinetics in colloidal hard spheres via real space analysis using Confocal microscopy — •Sahana Kale and Hans Joachim Schöpe — Institut für Angewandte Physik, Universität Tübingen, Germany

The nucleation rate densities from experimental and theoretical data diverge by several orders of magnitudes and the curves are qualitatively different. One of our research goals is to find the underlying reason for this discrepancy, if there is any.

Crystallization of meta-stable colloidal hard sphere suspensions is studied in real space using laser scanning confocal microscopy. Direct imaging in three dimension offers the unique possibility to observe crystal nucleation and growth on particle level giving detailed information about the fluid to crystal phase transformation

Keywords: Colloids, Confocal microscopy, Nucleation, Crystallization

CPP 17.22 Mon 17:30 Poster B1

Surface Preparation of Ice Single Crystals — •Markus Batzer[1,2], Jenée Cyran[1], Marc-Jan van Zadel[1], Ellen H. G. Backus[1,3], and Markus Mezger[1,2] — [1]Max Planck Institute for Polymer Research, Mainz — [2]Institute of Physics, Johannes Gutenberg University Mainz — [3]Department of Physical Chemistry, University of Vienna

Experiments in surface science often require samples made of high quality single crystals with surfaces containing little defects. However, at temperatures of around −10 °C, ice is a comparatively ductile material, making surface preparation challenging. We studied the near surface structure of ice single crystals prepared by different protocols using high resolution X-ray diffraction. Analysis of the diffraction data revealed that mechanical treatment can introduce distortions ranging up to several millimeters inside the bulk ice.

CPP 17.23 Mon 17:30 Poster B1

Post-treatment of thermoelectric polymer thin films to influence their thermoelectric properties — •Anna-Lena Oechsle, Nitin Saxena, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Thermoelectric materials are of great interest in terms of waste heat recovery and the use of solar thermal energy. Especially thermoelectric polymers are attractive, as they own some advantages over so far used inorganic thermoelectric materials, such as low cost, high mechanical flexibility, low or no toxicity, light weight and intrinsically low thermal conductivity. A way to evaluate the thermoelectric property of a material is the power factor $PF=S^2\sigma$. This parameter depends on the Seebeck coefficient S and the electrical conductivity σ, which again are affected by the electronic and morphological features of the polymer. In order to investigate ways to influence these features and improve the power factor, we fabricate thin semi-conducting polymer films and post-treat them in different ways. With measurements of the Seebeck coefficient, the electrical conductivity, UV-Vis, layer thickness changes and determination of the structure we attempt to find a morphology-function relation.

CPP 17.24 Mon 17:30 Poster B1

Electrically conductive multilayer films created from carbon nanotubes and polyelectrolytes — •Sven Neuber, Annekatrin Sill, Heiko Ahrens, and Christiane A. Helm — Institute of Physics, University of Greifswald, 17489 Greifswald, Germany

Films built from polyelectrolytes PSS, PDADMAC in 0.1 Mol/L NaCl and carbon nanotubes are investigated. Multilayer built-up was carried out by sequential adsorption of oppositely charged polyelectrolytes. Carbon nanotubes were modified with a volume/volume acid mixture (HNO3 (60-68%) and H2SO4 (98%)) to make them water soluble and negatively charged. AFM-images revealed a horizontal orientation of carbon nanotubes on the surface of the multialyer. Also, UV-vis, QCM and ellipsometry measurements were used to determinate surface coverage and thickness on nm-scale. Sheet resistance decreases monotonously with the number of carbon nanotube layers. Choosing the multilayer architectures allows to tune its sheet.

CPP 17.25 Mon 17:30 Poster B1

A new wafer scale deposition concept for 2D photoactive Bismuth/Bismuth(hydr)oxide multilayers for energy harvesting and environmental sensors — •Sebastian Runde, Christian von Savigny, and Christiane A. Helm — Institute of Physics, Universität Greifswald, Felix-Hausdorff-Str. 6, 17489 Greifswald

We present a transparent and photoactive multilayer consisting of ultrathin Bismut/Bismuth(hydr)oxide (Bi/BiOxHy) layers, prepared on glass substrates by induced break-up after forced wetting. A 3 nm thick monolayer is electrically isolating, transparent and laterally homogeneous. Multilayers are photoactive. The electric conductivity increases spontaneously with light intensity, it depends weakly on temperature and relative humidity. Thus, the sheet resistance can be tuned between 10 and 350 kΩ. To test long-term stability, the electric conductivity of the multilayer was measured in dependence of the local solar radiation. Fast-Fourier-Transformation of this time dependent sheet resistance shows a dominating cycle duration of ca. 24h.

CPP 17.26 Mon 17:30 Poster B1

Dynamics upon arrest in protein solutions with LCST phase behavior — •Anastasia Ragulskaya[1], Nafisa Begam[1], Anita Girelli[1], Hendrik Rahmann[2], Fajun Zhang[1], Christian Gutt[2], Thomas Zinn[3], and Frank Schreiber[1] — [1]Universität Tübingen — [2]Universität Siegen — [3]ESRF

Dynamically arrested states can occur as a result of an interplay of liquid-liquid phase separation (LLPS) and glass formation in protein and colloidal systems. We use a model system of bovine serum albumin (BSA) with YCl_3 which shows LLPS and a lower critical solution tem-

perature (LCST) phase behavior [1]. Following a temperature jump (T-jump) the protein-rich phase undergoes an arrested spinodal decomposition. Growth kinetics of a characteristic length as a function of time, observed using ultra-small angle X-ray scattering, shows a transition to an arrested state at high temperatures. Here, we investigate the dynamics of LLPS approaching the arrested state using X-ray photon correlation spectroscopy (XPCS). The analysis of two-time correlation functions obtained from XPCS shows compressed exponential dynamics in the temperature range $\sim 45-50$°C, with further transfer to stretched dynamics beyond 52.5°C. This may be treated as a transition from a superdiffusive to an intermittent dynamics of a glassy state. The dramatic jump of the characteristic relaxation time τ constant with q indicates the emergence of an arrested state above 52.5°C, but below thermal denaturation (60°C). For each T-jump, τ first increases, then becomes faster again before the system gets arrested.
[1] O.Matsarskaia et. al., *Phys. Chem. B*, **120**, 5564, 2016.

CPP 17.27 Mon 17:30 Poster B1

Heterogeneous dynamics in an arrested state in a protein system — •Anita Girelli[1], Nafisa Begam[1], Anastasia Ragulskaya[1], Hendrik Rahmann[2], Fabian Westermeier[3], Christian Gutt[2], Fajun Zhang[1], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]University of Siegen, Germany — [3]Petra III,DESY, Germany

In protein solutions, the interplay between LLPS and glass formation can lead to an arrested state. So far, little is known about the dynamic properties of the arrested state. Here we show the collective dynamics using XPCS for a protein-PEG system. The protein employed here is γ-globulin. PEG (polyethylene glycol) permits the attraction between the protein through depletion. The system has a upper critical solution temperature (UCST), and in a previous study the coarsening kinetics after quenching was studied with USAXS and USANS [1]. The results show that the size of the domains remains constant with time at very low temperatures (below glass transition) indicating that the system enters an arrested state. Here we find that the system close to the arrest shows lower relaxation times compared to the one where a complete phase separation occurs. The dynamics in the arrested state shows strong heterogeneity which increases with the quench depth. The results indicate the presence of cooperative domain motion, suggesting that the enhancement of cooperativity leads to the arrest at low temperatures.
[1] Da Vela et al., *Soft Matter*, **13**, 8756, 2017

CPP 17.28 Mon 17:30 Poster B1

Effect of shear on relaxation dynamics in glass-forming systems close to the glass transition — •Lawrence Smith, Dario Mauth, Gerhard Wilde, and Andreas Heuer — Westfälische Wilhelms-Universität, Münster, Germany

In ongoing experimental work on bulk metallic glasses, it has been observed that deformed samples may exhibit a higher relaxation enthalpy than an undeformed reference sample as measured by differential scanning calorimetry.

We investigate this effect using molecular dynamics (MD) simulations of a mixture of binary Lennard-Jones particles. The deformation of this model glass former is known to exibit a stress overshoot and shear-bands as observed in experimental bulk metallic glasses and is therefore appropriate to qualitatively reproduce these results and shed light on the underlying mechanisms.

The analysis of the underlying potential energy landscape of small systems has been shown to yield quantitative information on the systems dynamics in MD simulations in equilibrium. We use these same methods to investigate the relaxation from a deformed sample and an undeformed non-equilibrium sample close to the glass transition, and observe a crossing in the potential energy curves during relaxation.

Any anisotropy in the deformed sample vanishes before significant relaxation processes take place, ruling it out as a major factor on the relaxation. In larger samples we find a long lived local density modulation that may enable different mechanisms for the relaxation to take place in deformed and undeformed samples.

CPP 17.29 Mon 17:30 Poster B1

How coupled elementary units determine heterogeneity in macroscopic glass-forming systems — •Lawrence Smith and Andreas Heuer — Westfälische Wilhelms-Universität, Münster, Germany

Elementary units of a binary Lennard-Jones glassformer can be identified through quantitative analysis of its underlying potential energy landscape. These units can be fully understood within the continuous time random walk formalism and are found to contain the complete information concerning thermodynamics and diffusivity, while displaying finite size effects with respect to relaxation times and spacial correlations [1].

Previous research has shown that it is possible to identify major contributions to the non-Gaussian parameter as arising from the moments of the waitingtime distribution for jumps between metabasins of the potential energy landscape [2].

We investigate the impact of a coupling between elementary units on the non-Gaussian parameter (NGP) to gain insight into mechanisms underlying the emergence of dynamic heterogeneity as measured in the NGP and four-point correlation functions in the stochastic model as well as in molecular dynamics simulations.

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[2] C. Schröer, A. Heuer, *Phys. Rev. Lett.* **110**, 067801 (2013)

CPP 17.30 Mon 17:30 Poster B1

Impact of incorporating ultrastable glass layers on device efficiency and stability of organic light-emitting diodes — •Elisabeth Birgit Schwarz[1], Paul-Anton Will[1], Joan Ràfols-Ribé[2], Christian Hänisch[1], Marta Gonzalez-Silveira[2], Simone Lenk[1], Javier Rodríguez-Viejo[2], and Sebastian Reineke[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Germany — [2]Group of Nanomaterials and Microsystems, Universitat Autònoma de Barcelona, Spain

For current and future applications of organic-light emitting diodes (OLEDs), high device efficiency and stability are required. Additionally, to keep the process of making OLEDs competitive in the real production, simple device architecture and reproducibility are crucial. In this work, we present the incorporation of ultrastable glass layers in OLEDs as a concept that does not require material refinement or changes in stack architecture and is hence suggested to be generally applicable. At the same time, it allows to increase both, external quantum efficiency and lifetime of the OLEDs, by more than 15% compared to reference devices. This enhancement is achieved by fabricating several of the functional organic layers as ultrastable glasses through adjusting the substrate temperature and hence the growth conditions during physical vapor deposition. Ultrastable glasses appear as thermodynamically most favorable state and, thus, most stable molecular conformation in disordered solids achievable nowadays. We present detailed studies for OLEDs with four different phosphorescent emitters.

CPP 17.31 Mon 17:30 Poster B1

Multiple Glassy Dynamics of an Asymmetric PVME/PS Blend Investigated by Broadband Dielectric and Specific Heat Spectroscopy — •Paulina Szymoniak, Sherif Madkour, and Andreas Schönhals — Bundesanstalt für Materialforschung und prüfung (BAM), Berlin, Germany

Over the past decades research on the molecular dynamics of miscible polymer blends is of topical interest in the literature, to understand the segmental mobility of individual components, as it is affected by blending. In general, miscible polymer blends exhibit a complex dynamic behavior. For an A/B blend the relaxation times of component A and component B are affected by the spatial local compositional heterogeneity, present in binary systems on a microscopic level, regardless of the macroscopic homogeneity. Here, a combination of broadband dielectric and specific heat spectroscopy was employed to study the dynamically asymmetric PVME/PS blend with seven different compositions, focusing on samples with high PS contents. Considering that PS is dielectrically invisible, BDS is a powerful technique to study the response of PVME, as it is affected by PS segments. Here, three separate relaxation processes were found by dielectric investigations, related to confined or constrained PVME segments due to the spatial local compositional heterogeneities, which is in contrary to the previous literature findings [1]. Moreover, the dielectric data was compared with results obtained by specific heat spectroscopy, where a fourth relaxation process was found, due to the cooperative fluctuations of PVME and PS. [1] Colmenero, J., Arbe, A. Soft Matter, 2007, 3, 1474.

CPP 17.32 Mon 17:30 Poster B1

Tunable surprising glassy dynamics in MAPLE deposited nanostructured polymer — •Mithun Chowdhury[1], Xavier Monnier[2], Yucheng Wang[3], Daniele Cangialosi[2], and Rodney Priestley[3] — [1]Metallurgical Engineering and Materials Science, IIT

Bombay, Mumbai 400076, India — [2]Centro de Fisica de Materiales, CSIC-UPV/EHU, San Sebastian 20018, Spain — [3]Chemical and Biological Engineering, Princeton University, NJ 08544, USA

In this study we characterize glassy dynamics of Matrix Assisted Pulsed Laser Evaporation (MAPLE) deposited poly (methyl methacrylate) (PMMA) films. For that, we exploit fast scanning calorimetry to investigate the molecular mobility and the vitrification kinetics in terms of the thermodynamic state attained after a given cooling rate. We found in general any MAPLE deposited glass is thermodynamically more stable than bulk polymer standard glass, as indicated by lower fictive temperature in comparison to standard glass. Intriguingly, MAPLE deposited glasses exhibits at the same time faster molecular mobility. For a standard glass, the opposite behavior is generally found. Furthermore, by heating (aging and annealing) and controlling MAPLE deposition temperature, the amorphous state can be tuned. This still significantly deviates from the standard PMMA. We tentatively conclude that MAPLE deposited glasses are formed following a distinguished kinetic path, leading to an amorphous state well different from that of glasses formed in the conventional way, that is, by cooling through its glass transition temperature from melt.

CPP 17.33 Mon 17:30 Poster B1

Growth Kinetics and Molecular Mobility of Irreversibly Adsorbed Layers in Thin Polymer Films — •Marcel Gawek, Andreas Hertwig, 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 formed. These adsorbed layers have shown enormous potential for technological applications. The growth kinetics and molecular dynamics of these buried layers in thin films are still not fully investigated due to the hard accessibility. Here, the irreversibly adsorbed layers of homopolymer thin films are revealed by solvent-leaching experiments. 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) and spectroscopic ellipsometry. Additionally, the molecular mobility of the adsorbed layer is investigated with Broadband Dielectric Spectroscopy (BDS). A recently developed nanostructured capacitor (NSC) is employed to measure the adsorbed layers with a free surface layer depending on annealing and solvent-leaching time. The results are quantitatively compared and discussed with respect to recently published work.

CPP 17.34 Mon 17:30 Poster B1

Structure and morphology in tetracene-C60 blends — •Katja Schick, Clemens Zeiser, and Katharina Broch — Institut für Angewandte Physik, Universität Tübingen, Deutschland

Although C60 is one of the classical acceptors in organic solar cells [1], the mechanisms of its structure formation in blends are not fully understood. However, since the mixing behaviour or the length scales of phase separation are affecting device performance [2], an understanding of the underlying mechanisms is important. Phase separating systems can exhibit interesting kinetic effects as demonstrated, e.g. in blends of C60 and diindenoperylene (DIP), for which a thickness-dependent domain size has been observed [3].

In order to study how the length of the co-evaporated molecule influences the thickness-dependent phase separation and island size, we use tetracene (TET) which is shorter than DIP. To analyse the thickness-dependent structure and morphology of the TET:C60 films we use X-ray diffraction, AFM and SEM and discuss our findings in view of the steric compatibility of the two molecules.

[1] N. Martín et al. Chemical Review. 98(1998)
[2] S. Oosterhout et al. Nature Materials. 8(2009)
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CPP 17.35 Mon 17:30 Poster B1

Structural and optical properties of pentacene and tetracene blends — •Daniel Lepple, Clemens Zeiser, and Katharina Broch — Universität Tübingen

Optoelectronic devices based on organic semiconductors (OSCs) have found industrial applications, e.g. as light-weight and flexible displays [1]. In many devices, the active layer is composed of mixtures of two OSCs where one acts as a donor and the other one as an acceptor. As the device performance is strongly affected by the structural and optical properties of the mixed film, an understanding of structure-property relations is not only interesting from the viewpoint of fundamental research but also important for further device optimization. A prototypical class of OSCs to study the processes of structure formation and their impact on photophysical properties are acenes, especially tetracene and pentacene [2]. Although their properties have been studied extensively, there remain open questions due to the complex photophysics of these two molecules [3]. Here, we report on the structural and steady-state optical properties of blends of tetracene and pentacene, which we use as a model system for the study of structure-property relations in weakly interacting, structually compatible systems.

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[3] D. Beljonne et al. Physical Review Letter. 110 (2013)

CPP 17.36 Mon 17:30 Poster B1

Optical Investigation of Charge Transfer States in Tetracene/F6-TCNNQ Blends — •Christoph Theurer[1], Clemens Zeiser[1], Nico Hofeditz[2], Wolfram Heimbrodt[2], Martin Koch[2], and Katharina Broch[1] — [1]Eberhard Karls Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — [2]Philipps Universität Marburg, Physikalisches Institut, Renthof 5, Laborbau II, 35032 Marburg

Organic semiconductors have a huge potential for large area, cost and energy efficient optoelectronic devices like organic solar cells or OLED displays [1]. The majority of functional devices rely on charge transfer interactions between acceptor and donor molecules.

F6-TCNNQ is one of the strongest organic acceptor molecules known and is widely used for doping and studying charge transfer effects [2]. We have mixed it with tetracene, a member of the family of acenes, which exhibit interesting optical properties and effects like singlet fission [3]. Although tetracene is already intensively studied, little is known about charge transfer interactions in blends with acceptors [4]. We study the photophysics of the observed charge-transfer states and discuss our findings based on the structural and morphological properties of tetracene/F6TCNNQ blends with different mixing ratios. This serves as starting point for further time-resolved investigations of this fundamentally interesting system.

[1] Forrest, S. R., Nature 428 (2004) [2] Koech, P. K., et al., Chemistry of Materials 22 (2010) [3] Smith, M. B., and Michl, J., Chemical Reviews 110 (2010) [4] Hu, P., et al., CrystEngComm 19 (2017)

CPP 17.37 Mon 17:30 Poster B1

Analysis of metal nanostructure evolution on polymer surfaces by in-situ GISAXS during sputter deposition — •Valentin Munteanu[1], Simon J. Schaper[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[4], 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 — [4]KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden

A good understanding of the fabrication process of reproducible functional metal-polymer interfaces is of high importance for their use in organic electronics. Sputter deposition offers the ability to precisely control and tailor the fabrication of metal-polymer interfaces. During sputter deposition, the evolution of the metallic layer morphology is monitored in-situ with time-resolved grazing-incidence small-angle X-ray scattering (GISAXS). The resulting in-situ scattering data is processed and analyzed using the DPDAK software package. By fitting the processed data, structure parameters can be extracted whose temporal evolution reveals the mode of metal growth on polymer surfaces. Simulations with BornAgain lead to a deeper understanding of the growth mechanism of sputter deposited metal-polymer interfaces.

CPP 17.38 Mon 17:30 Poster B1

Self-assembly of large nanoparticles in ultrahigh molecular weight linear diblock copolymer films — •Wei Cao[1], Senlin Xia[1], Xinyu Jiang[1], Michael Appold[2], Matthias Opel[3], Markus Gallei[2], Matthias Schwartzkopf[4], Stephan V. Roth[4,5], 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 — [3]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — [4]DESY, Notkestrasse 85, 22603 Hamburg — [5]KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

The preparation of block copolymer nanocomposite films that consist of nanoparticles (NPs) with diameters (D) of more than 10 nm is a challenging task. Herein, ultrahigh molecular weight (UHMW) linear polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) diblock copolymer was spin-coated as a template for the self-assembly of large iron oxide NPs (D = 28.5 nm), and the morphology of hybrid nanocomposites was governed by the concentration (C) of the iron oxide NPs. Via hydrogen bonding between the carboxylic acid groups on iron oxide and the PMMA side chains of the diblock copolymers, the NPs were selectively incorporated inside the PMMA cylinders. Due to the rearrangement of the PMMA chains for accommodating the NPs, well-ordered cylindrical nanostructure were readily generated at low NP concentrations (C = 0.5 wt%). Most interestingly, a chain-like network appears inside the hybrid films at a high NP loading.

CPP 17.39 Mon 17:30 Poster B1

Thermal Oscillations in Homopolymer Blends — •Louis Pigard and Marcus Müller — Institute for Theoretical Physics, University of Göttingen, Germany

Immiscible homopolymer blends are binary mixtures that exhibit macroscopic phase-separation of their constituents A and B in equilibrium. The immiscibility of A and B is commonly characterized by the interaction parameter χN. For sufficiently high χN the blend demixes into two macroscopic A- and B-rich domains that are spatially separated by a single interface.

We study how this behaviour is altered if the temperature of the system and thus χN is oscillating in time. We model the dynamics by the Cahn-Hilliard equation and, additionally, verify our results with Monte-Carlo simulation of a soft, coarse-grained particle model that mimics Rouse dynamics.

For suitable values for the amplitude and period of the oscillation we observe the emergence of new metastable states with three interfaces and four domains in a thin-film geometry, i.e., the oscillation of incompatibility qualitatively changes the behavior from macro- to microphase separation in a thin film geometry.

We study the dependence of this microphase-separated state on the strength and frequency of the oscillation and explore the (meta)stability of the new, oscillation-induced state.

CPP 17.40 Mon 17:30 Poster B1

Free energy of interaction between polymers and Guanine-Quadruplexes using Molecular Dynamics Simulations — •Sanwardhini Pantawane and Stephan Gekle — Biofluid Simulation and Modeling Group, Theoretische Physik VI, Universität Bayreuth, 95440 Bayreuth Germany

In this investigation, free energy calculations on a system consisting of Poly(3-hexylthiopene-2,5diyl) (P3HT) chains and Guanine-Quadruplex DNA molecule, immersed in water are carried out. Such a polymer-DNA assembled system can be used to construct DNA biosensors, but has yet not been accomplised due to the lack of understanding of their conformational and thermodynamical stability. We construct a system with a four repeat G-Quadruplex molecule sitting over a planar surface of five collaterally arranged P3HT chains with 20 repeats each and apply umbrella sampling to pull the DNA molecule away from the P3HT polymer surface. We carry out the free energy calculations derived from a series of umbrella sampling simulations using a Weighted Histogram Analysis Method (WHAM), which would give an insight on determining the probability of the DNA molecule to attach to the conjugated polymers. An additional study on the effect of oxidation on such a G-quadruplex structures is also presented here.

CPP 17.41 Mon 17:30 Poster B1

Modelling DNA-strand displacement reactions in the presence of base-pair mismatches — •Patrick Irmisch and Ralf Seidel — Molecular Biophysics group, Peter Debye Institute for Soft Matter Physics, University of Leipzig, 04103 Leipzig, Germany

Toehold-mediated strand displacement is the most abundantly used method to achieve dynamic switching in DNA-based nanotechnology. A single-stranded 'invader' strand binds to the 'toehold' overhang of a target strand and replaces a target-bound 'incumbent' strand. Hereby, complementarity of the invader to the single-stranded toehold provides the energetic bias of the reaction.

The aim of this work is to obtain a quantitative description of the kinetics of strand displacement reactions in the presence of mismatches using simple biophysical modelling. This would allow for predicting strand-displacement rates when setting up strand-displacement reaction networks. We model the strand-displacement rate as the mean-first-passage time of a random walk within a simplified 1D energy landscape. In case of single invader mismatches, our model successfully describes the displacement kinetics as function of the mismatch position and the toehold length using a minimal set of parameters. Most importantly, our model is able to predict the kinetics of strand displacement reactions in presence of multiple invader mismatches as well as incumbent mismatches. Comparisons with experimental data confirm the model prediction and thus the general applicability of our approach.

CPP 17.42 Mon 17:30 Poster B1

Nano-electronic components built from DNA templates — •Jingjing Ye and Ralf Seidel — 1Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Germany

DNA Origami takes advantage of base complementarity of individual short oligonucleotides, to fold a long scaffold strand into almost any continuous 2D or 3D shape. We recently introduced a new concept of DNA origami mold-based particle synthesis that allows the synthesis of inorganic nanoparticles with a programmable shape. We demonstrated the concept by fabricating a 40 nm long rod-like gold nanostructure with a quadratic cross-section. We expanded the capabilities of the mold-based particle synthesis to demonstrate the synthesis of uniform μm long conductive gold nanowires with 20-30 nm diameters. With conductance characterization, metallic conducting wires were demonstrated. Here the concept is further expanded by designing mold monomers with different geometries and interfaces. We can fabricate more complex mold-superstructure in an addressable and flexible way like lego bricks.

CPP 17.43 Mon 17:30 Poster B1

Anomalous Diffusion in Reversible Networks — •Kiran Suresh Kumar[1,2], Jens-Uwe Sommer[1,2], and Michael Lang[1] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, Hohe Strasse 6, 01069 Dresden, Germany — [2]Institute für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01069 Dresden, Germany

Recent experiments and simulation studies find an anomalous super diffusive regime in reversible networks by analyzing Forced Rayleigh Scattering (FRS) data [1-3]. The molecular origin of this super diffusive regime is not yet fully understood. In our contribution, we approach this problem by computer simulations of FRS experiments in reversible networks based upon the Bond Fluctuation Model and additional stochastic simulations. We analyze the dynamics of individual molecules and correlate these with bond association and dissociation times. We further discuss the dependence of collective observables as accessible in FRS experiments with molecular parameters of the reversible gel.

[1] Tang, S.; Wang, M.; Olsen , B. D. J. Am. Chem. Soc. 2015, 137, 3946-3957.

[2] Tang, S.; Habicht, A.; Li, S.; Seiffert, S.; Olsen, B. D. Macromolecules 2016, 49, 5599-5608.

[3] Ramirez, J.; Dursch, T. J.; Olsen , B. D. Macromolecules 2018, 51, 2517-2525.

CPP 17.44 Mon 17:30 Poster B1

Investigation of swelling of coatings and the change of their mechanical properties at different air humidity — •Hannes Schedlberger[1], Bernhard Strauss[2], and Sabine Hild[1] — [1]Institute of Polymer Science, Johannes Kepler University Linz, Altenberger Str. 69, 4040 Linz, Austria — [2]Voestalpine Stahl GmbH, voestalpine-Straße 3, 4020 Linz, Austria

To protect steel surfaces against corrosion thin layer of organic coatings are applied. When used, water may be absorbed n the coatings and diffused through the layers. This can cause a variety of damages. Although this is a well known effect, the process of migration within the coatings and its consequences are still not clear. Therefore it is of utmost importance to investigate the amount of absorbed water, the adsorption kinetics and the correlation of the water absorption with the chemical structure and the mechanical properties of the coatings.

Atomic Force Microscopy (AFM) provides the possibility to observe the changes at the surface and to analyse the changes in the mechanical properties of the coatings as well. The swelling of the organic coating applied on a steel substrate were observed for 24 hours at various air humidity concentrations within a humidity cell at the AFM. To obtain the various air humidity concentrations, different salt solutions like potassium hydroxide or potassium nitrate were inserted into the humidity cell, followed by the analysis of the coatings. The changes of the mechanical properties of the coatings were analysed performing force distance curves.

CPP 18: Crystallization, Nucleation and Self-Assembly II (joint session CPP/BP)

Time: Tuesday 9:30–10:30 Location: H14

CPP 18.1 Tue 9:30 H14

Investigation of the Short-Time Diffusive Dynamics During Salt-Induced Protein Crystallization Using Neutron Spectroscopy — •Christian Beck[1,2], Marco Grimaldo[1], Felix Roosen-Runge[3], Fajun Zhang[2], Frank Schreiber[2], and Tilo Seydel[1] — [1]Institut Laue Langevin, Grenoble, France — [2]University of Tübingen, Germany — [3]Lund University, Lund, Sweden

Protein crystals are needed to obtain high-resolution protein structures, and therefore understanding different processes/pathways leading to their formation is of fundamental biophysical and medical interest. Previous studies investigating the kinetics of crystallization *in situ* using static methods (SAXS and microscopy) provided evidence for non-classical crystallization pathways in the presence of multivalent salts [1,2]. Using dissolved β-lactoglobulin proteins as a model system, we studied the $ZnCl_2$-induced crystallization. Here, we employ quasi-elastic neutron backscattering (NBS) and neutron spin-echo (NSE) spectroscopy to access the kinetics of the nanosecond diffusive dynamics of proteins during crystallization on a nanometer length scale. NBS provides information on the changes of the center-of-mass diffusion, internal diffusive dynamics and on the fraction of immobile proteins associated with the crystals. Accessing coherent scattering with NSE, we probe different scattering vectors q to disentangle the different diffusive contributions of proteins in crystals or aggregates, and in the liquid phase, respectively.

[1] A. Sauter *et al.* ACS Cryst. Growth Des. 14 (2014) 6357
[2] A. Sauter *et al.* Faraday Discuss. 179 (2015) 41

CPP 18.2 Tue 9:45 H14

Protein crystallization near liquid-liquid phase separation — Klim Petrov, Jan Hansen, •Florian Platten, and Stefan U. Egelhaaf — Heinrich Heine University Duesseldorf

The crystallization of protein (lysozyme) solutions is studied as a function of protein and salt concentration at ambient conditions. In addition to tetragonal crystals at low salt concentrations (far away from phase separation), needle-like and kinetically roughened crystals occur in the vicinity of the binodal. The crystallization induction time and the growth rate are inferred from optical microscopy and linked to the solubility and protein-protein interactions. Based on these data, the different states of the protein solution are linked to different driving forces for crystallization.

CPP 18.3 Tue 10:00 H14

Does liquid-liquid phase separation enhance protein crystallization? — •Ralph Maier[1], Andrea Sauter[1], Georg Zocher[1], Stefano Da Vela[1], Olga Matsarskaia[1], Ralf Schweins[3], Michael Sztucki[4], Fajun Zhang[1], Thilo Stehle[1,2], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Vanderbilt University School of Medicine, Nashville, USA — [3]ILL, Grenoble, France — [4]ESRF, Grenoble, France

Solutions of the protein human serum albumin (HSA) exhibiting a reentrant phase behavior with a metastable liquid-liquid phase separation (LLPS) inside the condensed regime in the presence of trivalent salts [1] were studied, focussing on the effects of the metastable dense liquid phase on the crystallization pathways. Optical microscopy and small angle X-ray and neutron scattering were used to follow protein crystallization and to explore the role of metastable LLPS. No evidence of nucleation inside the dense liquid phase was observed. On the contrary, heterogeneous nucleation at the walls of the glass container dominates. This suggests that the existence of a metastable LLPS is not a sufficient condition for a two-step nucleation. The unstable or metastable dense liquid phases serve as a reservoir for crystal growth. Furthermore, the crystallographic analysis of the resulting crystals shows that crystals with different morphology grown under different conditions share the same structure and the metal ions create two bridging contacts within the unit cell which stabilize the unit cell.
[1] Matsarskaia *et al.*, *J. Phys. Chem. B*, **120**, 7731 (2016)

CPP 18.4 Tue 10:15 H14

Using x-ray scattering to understand the formation of unexpected structures in organic thin films — Jenny Lebert[1], Eva M. Kratzer[1,2], Axel Bourdick[3], Mihael Coric[1], Stephan Gekle[3], and •Eva M. Herzig[1,2] — [1]Herzig Group, MSE Technische Universität München, Lichtenbergstr. 2a, 85748 Garching, Germany — [2]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [3]Biofluid Simulation and Modeling, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

The morphology plays an important role for the performance of organic, semi-conducting thin films. Understanding the self-assembly processes that occur during the drying of the photoactive films, will allow us to make progress in controlled nanomorphology tuning. We have therefore developed tools to investigate thin film formation processes using synchrotron radiation to resolve structure and structural developments [1,2]. We have now investigated an in-situ polymerization method for polythiophene to examine how much we can influence the morphology during film formation with such an approach. GIWAXS measurements, molecular dynamics simulations, and spectroscopic analysis suggest the presence of polythiophene in a novel and stable crystal structure with an enhanced intermolecular interaction [3]. [1] S. Pröller et al. Rev. Sci. Instrum. 2017, 88(6): 066101. [2] S. Pröller et al. Adv. Energy Mater. 2016, 6(1): 1501580. [3] J. Lebert et al. ACS Omega 2018, 6: 6388-6394.

CPP 19: Hybrid and Perovskite Photovoltaics II

Time: Tuesday 9:30–12:30 Location: H18

CPP 19.1 Tue 9:30 H18

Three-Terminal Perovskite Silicon Tandem Solar Cells with Top and Interdigitated Rear Contacts — •Philipp Tockhorn, Philipp Wagner, Johann Christoph Stang, Lukas Kegelmann, Mathias Mews, Steve Albrecht, and Lars Korte — Helmholtz Zentrum Berlin, Kekuléstraße 5, 12489 Berlin

So far, perovskite and silicon were paired in two terminal (2T) and four terminal (4T) tandems, yielding power conversion efficiencies (PCE) above 25 %. In a 2T tandem solar cell, the total current density is limited by the subcell yielding the lower current, restricting the overall performance. Independently operated 4T tandem cells need additional transparent conductive layers for lateral conduction and thus parasitic absorption is ultimately higher. Here, we present a novel three terminal (3T) approach for the interconnection of an n-i-p perovskite top cell with an interdigitated back contact (IBC) silicon heterojunction (SHJ) bottom cell. For this, the interconnection of the subcells is realised with SnO2 and nc-Si:H(n) layers. This allows the independent operation of both subcells in a monolithic device, thus combining the advantages of both 2T and 4T devices into a 3T tandem solar cell. For this, electrons generated in the perovskite top cell are collected at the rear side n-contact of the IBC SHJ. We report the first 3T perovskite/silicon tandem device in this architecture that reaches a combined stabilised PCE of 15.5 %. Despite losses due to hysteresis, our 3T device is still strongly limited by optical losses from high reflection and parasitic absorption. We present the theoretical limits of this tandem approach and highlight further routes to improve efficiency.

CPP 19.2 Tue 9:45 H18

Minimizing Electrical Interconnection Losses in Laser-Patterned Perovskite Solar Cells — •Markus Fenske[1], Christof Schultz[1], Andreas Bartelt[1], Antje Neubauer[2], Cornelia Junghans[2], Marko Jošt[3], Bernd Rech[4], Rutger Schlatmann[1,5], Steve Albrecht[3], and Bert Stegemann[1] — [1]Hochschule für Technik und Wirtschaft Berlin — [2]Becker & Hickl GmbH, Berlin — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Young Investigator Group for Perovskite Tandem Solar Cells — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, Institut für Silizium-Photovoltaik — [5]Helmholtz-Zentrum Berlin für Materialien und Energie, PVcomB

Successful up-scaling of metal halide perovskite (MHP) solar cells from lab-scale to large module sizes requires monolithic series interconnection. Here we report on recent progress in P2 and P3 laser patterning. By systematically varying the laser pulse energy, pulse duration and laser wavelength, a process window for the patterning could be established. We demonstrate the lateral effect of the laser processing on the chemical composition in the patterned area (by EDX) and on the perovskite semiconductor properties in the vicinity of the scribed laser line (by TR-PL). The results show that shorter laser pulse durations (ps rather than ns) and shorter laser wavelengths (355 nm rather than 532 nm) have a beneficial effect particularly on P2 process control, thereby minimizing electrical interconnection losses.

CPP 19.3 Tue 10:00 H18

Highly Efficient monolithic perovskite silicon tandem solar cells: analysing current-mismatch conditions — •Eike Köhnen, Marko Jost, Philipp Tockhorn, Anna B. Morales Vilches, Amran Al-Ashouri, Bernd Stannowski, and Steve Albrecht — Helmholtz-Zentrum Berlin, Germany

To well exceed the theoretical efficiency limit for silicon single junction solar cells, multiple absorbers with different bandgaps can be combined into tandem solar cells. Recently, metal halide perovskites have attracted significant scientific attention as tandem partner with silicon. Here, we combine a rear emitter silicon cell with a p-i-n perovskite cell into a highly efficient monolithic tandem cell. With this design, a certified tandem efficiency of 25% is realized at highly unmatched sub-cell photocurrents. Further improvements of the top contact and the perovskite thickness, enabled a remarkably efficiency of 26%, the highest yet published value. Additionally, we show how these tandem solar cells behave under various illumination spectra, e.g. when the sun spectrum changes over the day. Using selective illumination, different mismatch conditions are generated, affecting the tandem fill factor (FF). The experimental findings are reproduced by equivalent circuit simulations based on single cell parametrization. In both experiment and simulation, we find that the FF increases significantly when the sub-cells become more unmatched, an important finding as the FF enhancement slightly compensates the photocurrent reduction due to current mismatch. This will affect the mismatch condition for optimum performance and also affects the energy yield of the tandem solar cell.

CPP 19.4 Tue 10:15 H18

Characterisation of inorganic/hybrid lead and tin perovskites for efficient light-emitting diodes — •Ines Schmidt, Selina Olthof, and Klaus Meerholz — Universität zu Köln

Solution processable semiconducting perovskites have the general structure AMX_3, where A is a cation (Cs, methylammonium (MA) or formamidinium (FA)), M is a metal cation (Sn or Pb) and X is a halide anion (I, Br or Cl). The combination of these results in 18 different primary (i.e. non-mixed) perovskites with bandgaps corresponding to a wide range of the electromagnetic spectrum. This bandgap tunability, very narrow emission characteristic and a high charge carrier mobility make perovskites promising candidates for light-emitting applications.[1] To gain better understanding regarding possible emission wavelengths as well as the absolute energy levels, we optimized and characterized this complete set of 18 material combinations using structural, electrical and optical measurement techniques. With that knowledge, multi-layer perovskite light-emitting diodes with an optimized energy alignment can be fabricated. To this end, we introduced crosslinkable hole-transporting layers into the device stack to improve charge injection. Another important aspect is the enhancement of charge carrier recombination, which is typically done by reducing the grain size in perovskite films. Therefore, we investigated the impact of different small organic molecules and polymer additives in the preparation procedure on perovskite morphology and device performance.

[1] Stoumpos, C. C et al., Inorg. Chem., 52(15), 9019-9038 (2013).

CPP 19.5 Tue 10:30 H18

Pure Bromide-based Perovskites: Film Formation, Morphology and (In)Homogeneity — •Carolin Rehermann[1,2], Vincent Schröder[2], Sebastián Caicedo-Dávila[1], José Márquez Prieto[1], Aboma Merdasa[1], Emil List-Kratochvil[1,2] und Eva Unger[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, 12489 Berlin, Germany — [2]Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Due to their band gap tunability metal halide perovskites are an interesting material for tandem solar cells and LEDs, high band gaps around 2.3 eV are obtained with pure bromide perovskites.1 For established mixed perovskites wrinkled films are formed depending on preparation conditions. This inhomogeneity in composition and morphology influences the device performance.2, 3 Wrinkles develop likewise during preparation of pure bromides.

In this work, we study the film formation of organic and inorganic bromide-based perovskites with in-situ PL and UV/Vis measurements during different preparation steps and on various contact layers. Morphology and (In)homogeneity in composition of the final films are analyzed by XRD, PLimaging and EDX. Understanding parameters influencing wrinkle formation allows controlling this process and gives the opportunity to systematically provoke/ suppress them. That way resulting optoelectronic properties and detailed influences on device performance of wrinkles bromide perovskites are investigated.

1. Unger et al. Journal of Materials Chemistry A 2017, 5 (23), 11401-11409. 2. Braunger et al. J. Phys. Chem. C 2018, 122, 17123-17135. 3. Bercegol et al. J. Phys. Chem. C 2018, 122, 23345-23351.

CPP 19.6 Tue 10:45 H18

Methylammonium Lead Iodide Perovskite Solar Cells from direct Co-Evaporation — •Marcel Ross, Lidón Gil Escrig, Amran Al-Ashouri, Marko Jošt, and Steve Albrecht — Helmholtz-Zentrum Berlin, Young Investigator Group for Perovskite Tandem Solar Cells

Deposition of perovskite solar cell absorbers by co-evaporation offers a variety of advantages over solution based preparation such as homogeneous coating of large substrates and conformal coverage of textured substrates. Up to date the gas-like evaporation behavior of organic precursors such as methylammonium halides makes the rate measurement and consequently the process control difficult as volatile species might re-evaporate from chamber walls. To overcome these challenge we implement an evaporation setup with a thermal management system to directly co-evaporate volatile precursors for perovskites. Through a combination of actively cooled and heated surfaces, a direct and controlled evaporation process is achieved. This way, high quality Methylammonium Lead Iodide perovskite films are obtained as confirmed by XRD, PL and optical measurements. These perovskite films are implemented into p-i-n solar cells utilizing different hole transport materials (HTMs) such as PTAA, self-assembling monolayer (SAM) molecules and Spiro-TTB. Although the coarse grain morphology measured by SEM is very comparable, the solar cell performance is strongly affected by the used HTM and stabilized efficiency over 20% are realized with the SAMs only. The herein achieved efficiency is comparable to the highest reported value for evaporated perovskite solar cells.

CPP 19.7 Tue 11:00 H18

Structural and optical properties of $Cs_2AgBiBr_6$, a lead-free perovskite for photovoltaic applications — •Melina Armer[1], Julian Höcker[1], Liudmila Kudriashova[1], Sebastian Hammer[1], Kristofer Tvingstedt[1], Andreas Baumann[2], Jens Pflaum[1,2], and Vladimir Dyakonov[1] — [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 and stable lead-free materials for the application in perovskite photovoltaics has become an essential problem to be solved. In this work, lead-free $Cs_2AgBiBr_6$ single crystals have been synthesized using a solution based approach, permitting a detailed characterization of the optical and structural properties of this material. The single crystals have been characterized using steady-state and time-resolved photoluminescence (PL) spectroscopy. The morphology and quality of the as prepared crystals has been evaluated using scanning electron microscopy and X-ray diffraction. We observed PL in the visible region characterized by large time constants. Furthermore, $Cs_2AgBiBr_6$ thin films have been prepared and their optical and structural properties have been investigated, and compared to the corresponding bulk single crystals. Due to the encouraging optical and structural properties Cs$_2$AgBiBr$_6$ is a promising material for the application as absorber layer in lead-free perovskite solar cells.

15 min. break

CPP 19.8 Tue 11:30 H18

Improving the thermal stability of co-evaporated lead halide perovskites by replacing MA with Cs: Film growth and decomposition analyzed by *in situ* XRD — •Thomas Burwig, Paul Pistor, and Roland Scheer — Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle (Saale), Germany

Perovskites have seen a rising popularity in photovoltaic research due to their outstanding optoelectronic properties, with the most researched perovskite in this field being MAPbI$_3$. However, practical applications are held back by a lack of stability against atmospheric water, light and temperature. In our work we present fully inorganic caesium-lead-halide-perovskites, in which the organic MA is exchanged for caesium. We deposit thin films via dry, vacuum-based thermal co-evaporation. A specialized *in situ* X-ray diffraction setup allows us to monitor the crystal phase evolution over the course of the experiments. We report on the growth and thermally induced phase changes as well as the thermally induced decomposition of CsPbI$_3$ and CsPbBr$_3$ perovskites. CsPbI$_3$ is grown in a black, orthorhombic perovskite structure at room temperature (α'-CsPbI$_3$). This phase is stable in vacuum, but unstable under ambient conditions, as it undergoes a phase change to yellow, also orthorhombic δ-CsPbI$_3$. No such phase change was observed for CsPbBr$_3$. Our experiments confirm a higher thermal stability for CsPbI$_3$ and CsPbBr$_3$ as compared to the MA-lead-halides. Finally, we report on our attempts to synthesize further inorganic perovskites with improved stability.

CPP 19.9 Tue 11:45 H18

Kinetics of Ion-Exchange Reactions in Hybrid Organic–Inorganic Perovskite Thin Films Studied by In Situ Real-Time X-ray Scattering — •Alessandro Greco[1], Alexander Hinderhofer[1], M. Ibrahim Dar[2], Neha Arora[2], Jan Hagenlocher[1], Andrey Chumakov[3], Michael Grätzel[2], and Frank Schreiber[1] — [1]Institute for Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]Laboratory of Photonics and Interfaces, Institute of Chemical Sciences and Engineering, École Polytechnique Fédérale de Lausanne, Switzerland — [3]European Synchrotron Radiation Facility, 71, Avenue des Martyrs, CS 40220, 38043 Grenoble Cedex 9, France

The exchange of ions in hybrid organic–inorganic perovskites with the general formula APbX$_3$ (A = MA, FA; X = I, Cl, Br) is studied in five different systems using in situ real-time X-ray diffraction. In systems where the organic cation is exchanged, we find a continuous shift of the lattice parameter. The relative shift compared to the pure materials is used to quantify the exchange. Whether or not a conversion is possible, as well as the amount of exchanged cations, depends on the halide used. In the case of the interconversion of MAPbI$_3$ and MAPbCl$_3$, we observe a decay of the diffraction peaks of the original perovskite and the emergence of new peaks corresponding to the structure with the alternative halide. Moreover, we determined the relevant time scales of the growth and decay of the perovskite structures. [1]

[1] A. Greco *et al.*, J. Phys. Chem. Lett., **2018**, 6750 (DOI: 10.1021/acs.jpclett.8b02916)

CPP 19.10 Tue 12:00 H18

Manipulating the excited state of CsPbBr3 nanoplatelets for superior optical properties — •Thomas Morgenstern[1], Matthew Jurow[2,3], Carissa Eisler[2], Jun Kang[3], Manuel Engelmayer[1], Paul Alivisatos[2,3], Yi Liu[3], and Wolfgang Brütting[1] — [1]University of Augsburg, Institute of Physics, 86135 Augsburg, Germany — [2]College of Chemistry, University of California, Berkeley, California 94720, United States — [3]Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States

Lead halide perovskite (LHP) nanocrystals (NCs) and their light emitting features have recently moved into the focus of optoelectronic applications. However many properties of the nanoparticles remain to be investigated for a complete understanding of their optoelectronic attributes. Of crucial importance for lighting applications is the alignment of the emissive transition dipole moment with respect to the substrate normal, which limits the maximum achievable device performance. [1] To investigate this property we measured the photoluminescence radiation pattern of CsPbBr3 nanoplatelets. As a consequence of the nanocrystal shape, the energy of the emission peak shifts to shorter wavelengths, resulting in a deep blue emission maximum at 460 nm for the investigated nanoplatelets. Further the orientation of the transition dipole moments is confined in space and therefore aligns within the plane of the substrate. Hence the NCs have the potential to outperform existing solutions for blue emitting devices within display and lighting applications. [1] M. Jurow, et. al.: *Nano Lett.* **17(7)** (2017), 4534-4540

CPP 19.11 Tue 12:15 H18

Modeling MPa pressure-induced changes in photoluminescence spectra of organic-inorganic halide perovskites — Andrea Castelli[1], •Giulia Biffi[1,2], Luca Ceseracciu[1], Davide Spirito[1], Mirko Prato[1], Davide Altamura[3], Cinzia Giannini[3], Sergey Artyukhin[1], Roman Krahne[1], Liberato Manna[1], and Milena Arciniegas[1] — [1]Istituto Italiano di Tecnologia, Via Morego 30, 16163 Genova, Italy — [2]Dipartimento di Chimica e Chimica Industriale, Università degli Studi di Genova, Via Dodecaneso, 31, 16146, Genova, Italy — [3]Istituto di Cristallografia, Consiglio Nazionale delle Ricerche, via Amendola 122/O, 70126 Bari, Italy

High compressive strains have been used as a way to tune physical properties of three-dimensional perovskite crystals. Pressure in the GPa range generates structural distorsions in perovskite lattice, affecting the electronic structure and modifying optical and transport properties. Surprisingly, stacks of hybrid organic-inorganic perovskite flakes demonstrate tunability of optical spectra at much lower pressures, in the range of tens of MPa. Pristine flakes are near-white emitting, and in-situ photoluminescence experiments during loading and unloading in a mechanical pressure cell reveal drastic change in their optical emission spectrum, particularly an enhancement of the blue emission. Using first principles simulations, we are able to reproduce the main features of the optical properties and to analyze their variations under compressive strain.

CPP 20: Wetting, Fluidics and Liquids at Interfaces and Surfaces (joint session CPP/DY)

Time: Tuesday 9:30–13:00 Location: H13

CPP 20.1 Tue 9:30 H13

Non-monotonous wetting of graphene-mica and MoS$_2$-mica interfaces with a molecular layer of water — •Abdul Rauf, Andre Schilo, Nikolai Severin, Igor M. Sokolov, and Jürgen P. Rabe — Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Hydration of interfaces with a layer of water is a ubiquitous phenomenon. Nevertheless, the understanding of the wetting process is still limited, since it is experimentally difficult to follow. Here, graphene and monolayers of MoS$_2$ deposited on dry mica are used to investigate wetting of the 2D material-mica interfaces with a molecularly thin layer of water employing scanning force microscopy in different modes. Wetting starts at relative humidities (RH) of 10-17% for graphenes and 8-9% for MoS$_2$, and it concludes with a homogeneous layer at 25-30% and 15-20%, respectively. Wetting occurs non-monotonously in time and space for both types of interfaces. Initially a highly compliant and unstable layer of water spreads, which subsequently stabilizes by developing labyrinthine nanostructures. These nanostructures exhibit distinct mechanical deformability and dissipation, which is ascribed to different densities of the confined water layer. The laterally structured morphology is explained by the interplay of counteracting long-range dipole-dipole repulsion and short-range line tension, associated with the mechanical deformation of the 2D material. The proposed origins of the interactions are common for thin layers of polar molecules at interfaces, implying that the lateral structuring of thin wetting layers may also be a quite general phenomenon.

CPP 20.2 Tue 9:45 H13

Molecular Hydrophobicity at a Macroscopic Hydrophilic Surface — •Jenee D. Cyran[1], Michael Donovan[1], Doris Vollmer[1], Flavio Siro Brigiano[2], Simone Pezzotti[2], Daria R. Galimberti[2], Marie-Pierre Gaigeot[2], Mischa Bonn[1], and Ellen H.G. Backus[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]LAMBRE, Univ Every, Universite Paris-Saclay, Evry, France

Chemical and physical interactions between water and silicates are ubiquitous and relevant for geochemistry and industrial processes, including chromatography, oil extraction and coatings. Characterizing the silica/water interface is important to not only understand the fundamental properties for natural occurring processes but also to improve existing technologies, such as silica coatings, which rely on wettability and thermal-resistant properties to remain effective. At the silica/water interface, we compare the microscopic water organization, from both surface sensitive vibrational sum frequency generation experiments and molecular dynamics simulations, to macroscopic information about the hydrophobicity obtained from contact angle measurements. At the microscopic level, weakly hydrogen-bonded OH groups, typical for hydrophobic interfaces, are observed that originate from water molecules interacting with hydrophobic sites of the silica surface. Surprisingly, we observe the presence of hydrophobic water at a macroscopically hydrophilic water surface.

CPP 20.3 Tue 10:00 H13

Interfacial premelting of ice in nano composite materials — •Markus Mezger[1,2], Hailong Li[1], Julian Mars[1,2], and Markus Bier[3,4] — [1]Max Planck Institute for Polymer Research, Mainz — [2]Institute of Physics, Johannes Gutenberg University Mainz — [3]Max Planck Institute for Intelligent Systems, Stuttgart — [4]University of Applied Sciences Würzburg-Schweinfurt

The interfacial premelting in ice/clay nano composites was studied by high energy X-ray diffraction. Below the melting point of bulk water, the formation of liquid water was observed for the ice/vermiculite and ice/kaolin system. For the quantitative description of the molten water fraction in wet clay minerals we developed a continuum model for short range interactions and arbitrary pore size distributions. This model quantitatively describes the experimental data over the entire temperature range. Model parameters were obtained by fitting using a maximum entropy approach. Pronounced differences in the deviation from Antonow's rule relating interfacial free energy between ice, water, and clay are observed for the charged vermiculite and uncharged kaolin minerals. The resultant parameters are discussed in terms of their ice nucleation efficiency. Using well defined and characterized ice/clay nano composite samples, this work bridges the gap between studies on single crystalline ice/solid model interfaces and naturally occurring soils and permafrost.

[1] H. Li et al., Phys. Chem. Chem. Phys. DOI: 10.1039/c8cp05604h (2018)

CPP 20.4 Tue 10:15 H13

A Direct Inversion Approach to Local Permittivity at Liquid-Liquid Interfaces — •David Egger, Christoph Scheurer, and Karsten Reuter — Theoretische Chemie, TU München

Realistic models for catalytic reactions at liquid-liquid interfaces (LLIs) 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 reciprocal space formalism described by Neumann for wave-vectors at finite wavelength [1].

Exploiting the convolutional relation between dipole-dipole interaction tensor and polarization, we present a cavity kernel based approach in reciprocal space in order to arrive at local real space averages to calculate a spatially resolved $\varepsilon(\mathrm{r})$ from spheroidal gaussian cavities of different shape and volume, avoiding difficulties with geometry-induced boundary conditions in the electrostatic description. Results are discussed for water bulk and water-dichloroethane LLI systems.

[1] M. Neumann, Mol. Phys. 57:1, 97-121, 1986

CPP 20.5 Tue 10:30 H13

Testing dielectric continuum theory at interfaces by atomistic simulations — •Philip Loche[1], Cihan Ayaz[1], Alexander Schlaich[1,2], Douwe Jan Bonthuis[1], and Roland R. Netz[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Laboratoire Interdisciplinaire de Physique, CNRS and Université Grenoble Alpes, UMR CNRS 5588, 38000 Grenoble, France

Based on fully atomistic simulations of ions in water, we discuss the validity of continuum models for the dielectric response at aqueous interfaces. For the electrostatic energy of an ion in the vicinity of a hydrophobic graphene surface we find the electrostatic contribution to be dominated by the non-electrostatic contribution. Linear dielectric theory breaks down, and to quantitatively describe the linear dielectric contribution an anisotropic tensorial dielectric model is needed. This demonstrates the limitation of current continuum models for the dielectric response at interfaces.

Invited Talk CPP 20.6 Tue 10:45 H13

Dynamic surface tension of soft solids — Mathijs van Gorcum[1], Bruno Andreotti[2], Jacco Snoeijer[1], and •Stefan Karpitschka[3] — [1]University of Twente, Enschede, Netherlands — [2]Université Paris-Diderot, Paris, France — [3]MPI-DS, Göttingen, Germany

The contact line of a liquid drop on top of a solid surface exerts a nanometrically sharp surface traction, providing an unprecedented tool to study highly localized and dynamic deformations of soft polymer networks. The morphology is determined not only by bulk viscoelasticity, but also by solid surface tension. The latter may depend on strain, known as the Shuttleworth effect. Its impact on soft wetting is controversially discussed in recent literature. One of the outstanding problems in this context is the stick-slip instability of a moving contact line, which is observed above a critical velocity. Timeresolved measurements of the solid deformation are challenging, and the mechanism of dynamical depinning has remained elusive. Here we present direct visualizations of dynamic wetting ridges. Unexpectedly, the opening angle of the wetting ridge increases with speed, which cannot be attributed to bulk rheology. Instead, this effect points to an increase of solid surface tension not only in response to strain, but also depending on the rate of strain. Under this assumption, a criterion for depinning can be derived which is confirmed experimentally. We conclude that the surface tension of a solid is a truly dynamical quantity, following from a surface rheology that is different from the bulk, similar to what is known from liquid interfaces with surfactants.

15 min. break

CPP 20.7 Tue 11:30 H13

Raman spectroscopic evaluation of concentration gradients in small drops in binary mixtures on different substrates and in 3d printed small channels — •Alena Bell and Robert Stark — Physics of Surfaces, Materialwissenschaften, TU Darmstadt, Alarich-Weiss-Str. 16, 64287 Darmstadt, Deutschland

The evaluation of concentration gradients plays a big role in medical technology and chemotaxis. Microchannels are used in lab-on-chip devices for quick tests to test fluids directly, for example. Microchannels are also used for chemotaxis applications to mix fluids. The amount of liquid which is needed for these tests is in the microliter range. Raman spectroscopy is a powerful technique to detect changes in molecular structures within reactions in lab-on-chip devices and in chemotaxis devices. Therefore, different fluids are directed through 3d printed channels and changes are measured via Raman spectroscopy. In a first step, these generated fluid mixtures are measured as drops on different substrates. The concentration gradients that build up in the mixtures is measured in the drops. In the next step the gradients are measured in small channels. The concentration gradients are calculated by comparing relative peak intensities and correlating these results with calibration curves.

CPP 20.8 Tue 11:45 H13

Shallow water lattice Boltzmann simulations of thin film flows — •Stefan Zitz[1], Andrea Scagliarini[2], Suryanarayana Maddu Kondaiah[3], Anton Darhuber[4], and Jens Harting[1,4] —

[1]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Nürnberg, Germany — [2]Institute for Applied Mathematics "M. Picone" (IAC-CNR), Rome, Italy — [3]Center for System Biology (MPI-CBG), Dresden, Germany — [4]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

We propose a novel approach to the numerical simulation of thin film flows, based on the viscocapillary shallow water equations. The integration is performed by the means of a suitably devised lattice Boltzmann method.

The numerical scheme is applied to the viscous Rayleigh-Taylor instability of a thin film under the influence of gravity as well as the spreading of a sessile drop towards its equilibrium contact angle. During the spreading we observe a linear correlation between the spreading speed and the contact angle, as theoretically predicted by the Cox-Voinov law.

Further we address the problem of a droplet sliding on an inclined plane. Due to the choice of the substrate friction we observe a pinning region for low forcing. When increasing the forcing by varying the droplet volume the droplet starts to slide and the Capillary number scales linearly with the Bond number.

CPP 20.9 Tue 12:00 H13

Complex Wetting: flow profiles close to three phase contact lines — •Benedikt Straub[1], Franziska Henrich[1], and Günter K. Auernhammer[2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Leibniz Institute for Polymer Research, Dresden, Germany

Wetting and dewetting behavior on solid surfaces is the crucial process underlying many natural phenomena as well as technical applications like printing or coating of surfaces. Our aim is to study the wetting behavior of surfactant solutions on solid surfaces. Especially the flow profile close to the three phase contact line is highly interesting for modelling efforts.

Three-dimensional flow profiles are measured with an astigmatism particle tracking velocity setup.

Measurements of a receding contact line for pure water show that the theoretical prediction can be reproduced, which is used to validate the system. First results show that surfactants cause a deviation of the flow field in comparison to theoretical predictions for pure liquids. In the case of a receding contact line new air-liquid interface is formed at the three phase contact line. The freshly formed interface is, in comparison to the already existing air-liquid interface, not completely occupied by surfactants. This causes a Marangoni tension in the direction of the contact line along the interface. This Marangoni tension opposes the bulk flow close to the air-liquid interface and causes a deviation of the flow field. In special cases this can lead to an opposing interface flow compared to the bulk flow.

CPP 20.10 Tue 12:15 H13

Direct observation of gas meniscus formation on a superhydrophobic surface — •Doris Vollmer[1], Mimmi Eriksson[2], Agne Swerin[2], Hannu Teisala[1], Michael Kappl[1], and Hans-Jürgen Butt[1] — [1]MPI for Polymer Research, Mainz, Germany — [2]RISE Research Institutes of Sweden, Stockholm, Sweden

The formation of a bridging gas meniscus via cavitation or nanobubbles is considered the most likely origin of the long-range attractive forces measured between hydrophobic surfaces in aqueous solution. On a superhydrophobic surface a thin air layer is present and influences the interaction. Here, we report time and space resolved imaging of the formation and growth of a gas meniscus during force measurements between a superhydrophobic surface and a hydrophobic microsphere immersed in water. This is achieved by combining laser scanning confocal microscopy and colloidal probe force microscopy. The configuration allows determination of the volume and shape of the meniscus, together with direct calculation of the Young-Laplace capillary pressure. The long-range attractive interactions acting on separation are due to meniscus formation and volume growth as air is pulled from the surface layer.

CPP 20.11 Tue 12:30 H13

Wetting of n-Alkane Nano-Patterns: Evidence of Macroscopic Line Tension Effects and Adaptive Wetting — •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 wetting study of silicon samples coated with a single layer of n-alkane molecules self-assembled perpendicular to the surface by velocity-dependent dip-coating. The contact angle was measured with 2 microliters of ultrapure water for different n-alkane surface coverages. The results of the apparent contact angle versus coverage can be grouped in two regimes that depend linearly on coverage. This can be described by the Cassie wetting model along with the consideration of line tension effects. The two wetting regimes are characterized by two line tensions representing distinct alkane monolayer morphologies, i.e. dentritic and stripe patterns resulting from different dip-coating velocities. During drop evaporation, there is a restructuring of the alkane monolayer structure which could be related to adaptive wetting. Acknowledgements: FONDECYT Nos. 3160803 (MJR), 1180939 (UGV) 1171047 (MSA) and 11160664 (TPC), CONICYT Fellowship (MC) and CONICYT-PIA ACT 1409.

CPP 20.12 Tue 12:45 H13

Impact of Nanoparticles' Surface Properties on their Physico-Chemical Behavior in Pickering Emulsions — •Sebastian Stock, Dmitrij Stehl, Sandra Forg, and Regine von Klitzing — TU Darmstadt, Darmstadt, Germany

Pickering Emulsions (PEs) were first studied by S. U. Pickering in the beginning of the last century and describe emulsions stabilized by particles that adsorb at the oil water interface and prevent coalescence of the droplets. In the present study Halloysite Nanotubes, fumed colloidal silica and Latex nanospheres are used to stabilize PEs. They display significant differences regarding their surface properties, size and shape. The surface of these particles is modified in order to investigate the influence of surface charge or hydrophobicity on the whole systems behavior including emulsion stability and reaction performance in homogeneous catalysis at the oil-water-interface. Additionally, the effect of the surface-active Rh-catalyst is investigated. The interaction between catalyst and particle surface plays a significant role for mass transfer and conversion.

CPP 21: Two-dimensional Materials I (joint session HL/CPP)

Time: Tuesday 9:30–13:00 Location: H36

CPP 21.1 Tue 9:30 H36

Electronic Dipole Spin Resonance of 2D Semiconductor Spin Qubits — •Matthew Brooks and Guido Burkard — Universität Konstanz, Konstanz, Deutschland

Monolayer transition metal dichalcogenides (TMDs) offer a novel two-dimensional platform for semiconductor devices. One such application, whereby the added low dimensional crystal physics (i.e. optical spin selection rules) may prove TMDs a competitive candidate, is quantum dots as qubits. The band structure of TMD monolayers offers a number of different degrees of freedom and combinations thereof as potential qubit basis, primarily electron spin, valley isospin and the combination of the two due to the strong spin orbit coulping known as a Kramers qubit. Pure spin qubits in monolayer $\mathrm{Mo}X_2$ (where $X =$ S or Se) have been shown to be achievable by energetically isolating a single valley and tuning to a spin degenerate regime within that valley by a combination of a sufficiently small quantum dot radius and large perpendicular magnetic field. Within such a TMD spin qubit, we theoretically induce and analyse single qubit rotations with an electric dipole spin resonance. We employ a rotating wave approximation within a time dependant Schrieffer-Wolf approximation to derive analytic expressions for the Rabi frequency of single qubit oscilations, and compare this result to more exact numerics, as to find optimal operational regimes.

CPP 21.2 Tue 9:45 H36

Metalorganic Vapour Phase Epitaxy (MOVPE) Technology for 2D Transition Metal Dichalcogenides (TMDC) — •Michael Heuken[1,2], Annika Grundmann[2], Dominik Andrzejewski[3], Tilmar Kümmell[3], Gerd Bacher[3], Holger Kalisch[2], and Andrei Vescan[2] — [1]AIXTRON SE, Dornkaulstr. 2, 52134 Herzogenrath, Germany — [2]Compound Semiconductor Technology, RWTH Aachen University, Sommerfeldstr. 18, 52074 Aachen, Germany — [3]Werkstoffe der Elektrotechnik and CENIDE, University Duisburg-Essen, Bismarckstr. 81, 47057 Duisburg, Germany

The 2D TMDC $\mathrm{MoS_2}$ and $\mathrm{WS_2}$ have raised strong interest due to their exceptional properties and prospects for micro- and optoelectronics. For fundamental material physics and the development of (opto)electronic devices, a reproducible deposition technology providing uniform layers of controlled thickness and purity is indispensable. MOVPE is perfectly suited for this task and can furthermore be scaled up to production with high volume and yield. Here, we report on the systematic investigation of 2D $\mathrm{MoS_2}$ and $\mathrm{WS_2}$ growth on sapphire using a hydride-free MOVPE process in a commercial AIXTRON multiwafer MOVPE reactor. Metal hexacarbonyls (WCO and MCO) as well as DTBS are used as high-purity MO sources. The impact of the fundamental growth parameters is discussed, shedding light on nucleation and lateral 2D growth until full layer coalescence. Samples are characterized using Raman spectroscopy, SEM, AFM, PL, and reflectometry. Finally, a $\mathrm{WS_2}$-based LED will be presented to demonstrate the applicability of 2D TMDC for optoelectronic devices.

CPP 21.3 Tue 10:00 H36

Interplay of bright and dark excitons in transition metal dichalcogenides — •Malte Selig[1], Dominik Christiansen[1], Florian Katsch[1], Ermin Malic[2], and Andreas Knorr[1] — [1]Nichtlineare Optik und Quantenelektronik, Institut für Theoretische Physik, Technische Universität Berlin, Deutschland — [2]Chalmers University of Technology, Department of Physics, Göteborg, Sweden

The extraordinarily strong Coulomb interaction in monolayers of transition metal dichalcogenides (TMDs) gives rise to the formation of tightly bound electron hole pairs, excitons, which dominate the optical and electronic properties of these ultrathin materials. In particular, a variety of dark exciton states occurs, including excitons with opposite spins of the constituent carriers [1] and excitons with momenta well above the radiative cone [2]. In this talk, we will address the impact of such dark exciton states to the optical properties of TMDs, including optical lineshape [2,3], luminescence properties [4] and intervalley relaxation. Additionally, we compare the influence of these states on the excitonic linewidth between mono- and bilayer samples [5].

[1] X.-X. Zhang et al., Nature Nanotechnology 12, 883 (2017)
[2] M. Selig et al., Nature Communications 13279 (2016)
[3] D. Christiansen et al., Physical Review Letters 119, 187402 (2017)
[4] M. Selig et al., 2D Materials 5 035017 (2018)
[5] A. Raja et al., Nano Letters, 18 (10), 6135 (2018)

CPP 21.4 Tue 10:15 H36

Many-body quantum Monte Carlo study of 2D materials: cohesion and band gap in single-layer phosphorene — •Tobias Frank[1], Rene Derian[2], Kamil Tokar[2], Lubos Mitas[3], Jaroslav Fabian[1], and Ivan Stich[2,4] — [1]University of Regensburg, Regensburg, Germany — [2]Slovak Academy of Sciences, Bratislava, Slovakia — [3]North Carolina State University, Raleigh, NC — [4]University of Ss. Cyril and Methodius, Trnava, Slovakia

Quantum Monte Carlo (QMC) is applied to obtain the fundamental (quasiparticle) electronic band gap, Δ_f, of a semiconducting 2D phosphorene. Similarly to other 2D materials, the electronic structure of phosphorene is strongly influenced by reduced screening, making it challenging to obtain reliable predictions by conventional methods. Using the recently uncovered universal scaling between the exciton binding energy and Δ_f, we predict the optical gap of about 1.7 eV that can be directly related to experiments. The QMC gaps agree with recent optical absorption and photoluminescence measurements. We also predict the cohesion of phosphorene to be only slightly smaller than that of the bulk crystal. Our investigations not only benchmark GW methods and experiments, but also open the field of 2D electronic structure to computationally intensive but highly predictive QMC methods which include many-body effects such as electronic correlations. We were supported by GRK Grant No. 1570, the International Doctorate Program Topological Insulators of the Elite Network of Bavaria, and DFG SFB 1277 (B07). We acknowledge the Gauss Centre for Supercomputing (www.gauss-centre.eu) for funding.

CPP 21.5 Tue 10:30 H36

Interlayer band-to-band tunneling in h-BN encapsulated MoS2-WSe2 heterojunction — •Phanish Chava[1,2], Vivek Mootheri[1], Himani Arora[1,2], Kenji Wantanbe[3], Takashi Taniguchi[3], Manfred Helm[1], and Artur Erbe[1] — [1]Helmholtz Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328 Dresden, Germany — [2]TU Dresden, 01062 Dresden, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

Quantum mechanical band-to-band tunneling (BTBT) is a particular type of carrier injection mechanism which is responsible for the electronic transport in tunneling based devices like Esaki diode and Tunnel Field Effect Transistor (TFET). Atomically thin layers of transition metal dichalcogenides (TMDCs) are promising semiconducting materials for realizing such devices owing to their sharp interfaces. In this work, we demonstrate BTBT between the layers of molybdenum disulfide (MoS2) and tungsten diselenide (WSe2) in a MoS2-WSe2 heterojunction which is encapsulated with hexagonal boron nitride (h-BN) on the top and bottom. Also, we employ few-layer graphene as the contact material to the heterojunction thereby forming a 2D-2D van der Waals contact. We find that the device works as a p-TFET for for negative top gate voltages and an n-MOSFET for positive top gate voltages. The device exhibits Negative Transconductance (NTC) in the positive gate voltage regime, a minimum sub-threshold swing of about 170 mV / dec at 125 K and an ON-OFF ratio of about 10^6.

CPP 21.6 Tue 10:45 H36

Effects of the Fermi Level Energy on the Adsorption of O2 to Monolayer MoS2 — •Philip Klement[1], Christina Steinke[3], Sangam Chatterjee[1], Tim Wehling[3], and Martin Eickhoff[2] — [1]Institute of Experimental Physics I and Center for Materials Research, Justus Liebig University Giessen, D-35392 Giessen, Germany — [2]Institute of Solid State Physics, University of Bremen, D-28359 Bremen, Germany — [3]Institute for Theoretical Physics and Bremen Center for Computational Material Sciences, University of Bremen, D-28359 Bremen, Germany

Two-dimensional transition metal dichalcogenides possess large surface-to-volume ratios that make them ideal candidates for sensing applications such as detecting the surface adsorption of specific gas molecules. The resulting changes of the electrical and optical properties allow for detection and analysis of interaction mechanisms at the sensing interface. Specifically, we investigate the influence of O2 adsorption on monolayer MoS2 and the role of the Fermi level energy in this process. We record the response in photoluminescence and transport properties of monolayer MoS2 upon O2 adsorption and the impact of external electric gating. We find an increase of the photoluminescence intensity and a reduction of the conductivity upon O2 adsorption, and show that the adsorption can be enhanced by an increase of the Fermi level energy. These results demonstrate that ionosorption of O2 on MoS2 by charge transfer only occurs if free carriers are available in the conduction band of MoS2. Furthermore, photoluminescence recording is rendered advantageous for sensing.

15 min. break

CPP 21.7 Tue 11:15 H36

Zeeman splitting and inverted polarization of biexciton emission in monolayer WS$_2$ — •Philipp Nagler[1], Mariana V. Ballottin[2], Anatolie A. Mitioglu[2], Mikhail V. Durnev[3], Takashi Taniguchi[4], Kenji Watanabe[4], Alexey Chernikov[1], Christian Schüller[1], Mikhail Glazov[3], Peter C. M. Christianen[2], and Tobias Korn[1] — [1]University of Regensburg — [2]High Field Magnet Laboratory, Nijmegen — [3]Ioffe Institute, St. Petersburg, Russia — [4]NIMS, Tsukuba, Japan

Monolayer TMDCs are an ideal testbed to study the physics of quasiparticles in the two-dimensional limit. Besides excitons, more complex many-body states such as trions and biexcitons can emerge due to the strong Coulomb interaction in these materials. Here, we shed light on the intricate many-body physics of biexcitons in monolayer WS$_2$ [1]. The encapsulation of the monolayer between two sheets of hBN significantly reduces the overall spectral broadening and allows us to observe biexciton emission with linewidths below 5 meV at 4 K. In magneto-PL experiments, we observe an inverted field-induced polarization, implying a preferential population of the high-energy peak in emission. We explain this unusual phenomenon by considering the evolution of the total energy of the biexciton complex in a magnetic field. Based on the experimental results and the developed model we are able to identify the momentum-space configuration of the optically dominant biexciton state of monolayer WS$_2$.

[1] P. Nagler et al., *Phys. Rev. Lett.* **121**, 057402 (2018)

CPP 21.8 Tue 11:30 H36

Electromagnetically induced transparency in second-harmonic generation from monolayer WSe2 — •Kai-Qiang Lin, Robert Martin, Sebastian Bange, and John Lupton — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93053 Regensburg, Germany

Electromagnetically induced transparency (EIT) occurs in atomic systems and shows versatile applications in slow-light generation, gain without inversion and optical quantum-information processing. We demonstrate a cavity-free, atomic-like EIT effect in single-layer crystals of WSe2, probed by exploiting the intrinsic second-harmonic generation (SHG) arising from the breaking of inversion symmetry.[1] Under conditions of double resonance of the driving and radiated field with the fundamental transitions, the SHG spectrum bifurcates. The feature follows a pump-wavelength-dependent spectral anticrossing, accurately described by a ladder-type three-level model. Crucially, the SHG power-law exponent diverges from the canonical value of 2 to follow a Fano-like dispersion with wavelength. This dispersion is retained at room temperature, implying persistence of quantum interference. Our work opens up opportunities to exploit quantum nonlinear optics such as inversionless gain in the solid state.

[1]. K.-Q. Lin, S. Bange and J. M. Lupton, Nature Physics, in press. (preprint: https://arxiv.org/abs/1811.09479)

CPP 21.9 Tue 11:45 H36

Studying exciton-phonon interaction in a MoSe$_2$ monolayer by fluorescence-detected 2D electronic micro-spectroscopy — •Donghai Li[1], Chiara Trovatello[2], Stefano Dal Conte[2], Matthias Nuss[1], Giancarlo Soavi[3], Andrea Ferrari[3], Giulio Cerullo[2,4], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Dipartimento di Fisica, Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Milano, Italy — [3]Cambridge Graphene Centre, University of Cambridge, Cambridge, UK. — [4]Istituto di Fotonica e Nanotecnologie, CNR, Piazza Leonardo da Vinci 32, 20133 Milano, Italy

Monolayer transition metal dichalcogenides (TMDs) received extensive attention as they have extraordinary opto-electronic characteristic. Exciton-phonon interaction in TMD monolayers can result in sidebands in their absorption spectra, for some dark states are activated by exciton-phonon scattering [1]. However, in the absorption spectra, the phonon-induced sidebands are obscured by inhomogeneous broadening. Here, we study the excitonic physics of a MoSe$_2$ monolayer using fluorescence-based two-dimensional (2D) electronic spectroscopy. We confirm and extend the theoretical prediction [1] by our observations of sidebands and their quantum beating behavior within the 2D spectra. The analysis indicates a four-level energy structure with one dark state near the excited state and an additional, unpredicted, one near the ground state activated by exciton-phonon scattering.

[1] D. Christiansen et al., Phys. Rev. Lett. **119**, 187402 (2017)

CPP 21.10 Tue 12:00 H36

Transport and photoelectron spectroscopy of few-layer epitaxial WSe$_2$ — •Hiro Nakamura[1], Avaise Mohammed[1], Philipp Rosenzweig[1], Kathrin Müller[1], Peter Wochner[1], Armin Schulz[1], Mona Stadler[2], Michael Jetter[2], Peter Michler[2], Ulrich Starke[1], and Hidenori Takagi[1,3,4] — [1]Max Planck Institute for Solid State Research — [2]Institut für Halbleiteroptik und Funktionelle Grenzflächen, University of Stuttgart — [3]Department of Physics, University of Tokyo — [4]Institute for Functional Matter and Quantum Technologies, University of Stuttgart

Giant spin splitting of monolayer WSe$_2$ is an interesting element both for spintronics and topological phenomena. Here, we present electronic and structural properties of few-layer WSe$_2$ grown by hybrid pulsed-laser deposition. Angle-resolved, ultraviolet and X-ray photoelectron spectroscopy reveal the band structure of monolayer WSe$_2$ including strong spin-orbit splitting, as well as clarify the band alignment between WSe$_2$ and the underlying graphene/SiC substrate, indicating electron transfer from graphene to WSe$_2$. To access the valence bands in transport, hole-doping of few-layer WSe$_2$ has been performed using Nb as a dopant. The Hall effect and transport measurements confirmed the expected density of hole carriers, and associated metallic conduction down to low temperatures for optimal films. Synchrotron X-ray diffraction sheds further light on structure-property relationships, in particular strain effects in the WSe$_2$ layer.

CPP 21.11 Tue 12:15 H36

Excitation-Induced Transition from Direct to Indirect Band Gaps in Monolayer TMDs — •Daniel Erben[1], Alexander Steinhoff[1], Michael Lorke[1,2], Tim Wehling[1,2], Christopher Gies[1], and Frank Jahnke[1] — [1]Institute for Theoretical Physics, University of Bremen — [2]Bremen Center for Computational Materials Science, University of Bremen

Monolayers of transition metal dichalcogenides (TMDs) show exceptionally strong Coulomb interaction between charge carriers due to the small thickness and weak dielectric screening. Many-body interactions induced by excited charge carriers directly influence the electronic and optical properties in these materials. Strong many-particle renormalizations caused by the Coulomb interaction of the excited carriers will be discussed for MoS$_2$, MoSe$_2$, WS$_2$ and WSe$_2$. We solve the semiconductor Bloch equations on the full Brillouin zone using ab-initio band structures and interaction matrix elements.

Large excitation-dependent band-gap renormalizations are found. In all four materials, the conduction band Σ-valley exhibits a stronger shift to lower energies than the K-valley. As a result, all four TMDs show a tendency to become more indirect or even undergo a transition from a direct to indirect band gap with increasing excited carrier density.

For optical excitation of monolayer TMDs, we also study the connection between pump fluence and excited carrier density. The contributions of various many-body effects to a strong non-linearity are identified.

CPP 21.12 Tue 12:30 H36

Theory of Exciton-Exciton Coupling in Atomically Thin Transition Metal Dichalcogenides — •Florian Katsch, Malte Selig, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, 10623 Berlin, Germany

The valley-selective circular dichroism in monolayer transition metal dichalcogenides (TMDCs) and the subsequent fast valley depolarization due to intervalley Coulomb interactions enables the study of new many-body physics in these atomically thin materials. Here, a microscopic approach is presented to describe the optical response of monolayer TMDCs dominated by strongly correlated, bound electron-hole pairs [1, 2]. The approach includes Hartree–Fock and correlation effects up to two excitonic excitations [3], as well as TMDC typical Coulomb intra- and intervalley coupling and exciton-phonon interactions [4]. The developed theory is applied to access the exciton dynamics in the coherent limit and contributes to the understanding of valley-selective pump-probe experiments [5, 6].

[1] A. L. Ivanov and H. Haug, *Phys. Rev. B* **48**, 1490 (1993).
[2] F. Katsch et. al., *Phys. Status Solidi B*, 1800185 (2018).
[3] V. M. Axt and A. Stahl, *Z. Phys. B* **93**, 2 (1994).
[4] M. Selig et. al., *2D Mater.* **5**, 035017 (2018).
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[6] R. Schmidt et. at., *Nano Lett.* **16**, 2945 (2016).

CPP 21.13 Tue 12:45 H36

Creation and optical spectroscopy of localized excitons in 2D MoS_2 — •Oleg Gridenco, Sven Mehrkens, Kathrin Sebald, Christian Tessarek, Martin Eickhoff, and Jürgen Gutowski — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, D-28359 Bremen, Germany

It is known that missing atoms in a semiconductor are exciton trapping sites, moreover, excitons can bind to impurity atoms or can be trapped in a potential well created by local strain or structural defects. In this context, structuring with a focused ion beam gives the opportunity for manipulation of 2D materials on the nanometer scale. In this study, we explore how focused gallium ion irradiation affects the intrinsic luminescence and vibrational properties of atomically thin MoS_2. Defects were introduced by scanning the Ga^+ ion probe over a certain area of the flake using a focused ion beam (FIB). The amount of defects was controlled by varying the Ga^+ ion dose starting from 2 x 10^{12} ions/cm^2 until the PL signal was completely vanished (2 x 10^{13} ions/cm^2). After Ga^+ ion irradiation, micro-photoluminescence measurements at T=4K show that the A exciton emission is suppressed and a new peak, a bound exciton (D) located at 1.75 eV, emerges. This broad peak is redshifted by $\Delta E \sim 170$ meV with respect to the neutral exciton X emission. Encapsulating monolayer MoS_2 into hBN drastically reduces the inhomogeneous contributions to the exciton linewidth [1]. The possibilities of tailoring optically active defect centers in 2D MoS_2 to even host single-photon emitters will be discussed.

[1] E. Courtade et al., Appl. Phys. Lett. **113**, 032106 (2018).

CPP 22: Plasmonics I (joint session O/CPP)

Time: Tuesday 10:30–12:45 Location: H8

CPP 22.1 Tue 10:30 H8

Creating functional plasmonic fields with orbital angular momentum via meta structures — •Eva Prinz[1,2], Grisha Spektor[3], Michael Hartelt[1], Anna-Katharina Mahro[1], Meir Orenstein[3], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany — [3]Department of Electrical Engineering, Technion - Israel Institute of Technology, Israel

Optical fields can carry spin angular momentum (SAM) in the form of circularly polarized light and orbital angular momentum (OAM) as helical wavefronts. In the field of plasmonics, surface plasmon polaritons (SPPs) can carry surface confined OAM in the form of plasmonic vortices. Controlling such vortices opens the door towards a variety of applications.

Plasmonic OAM can be generated by the use of plasmonic vortex lenses (PVLs), a type of coupling structure based on Archimedean spirals. We demonstrate both experimentally and in simulations a modular plasmonic lens assembling strategy for the sculpturing of functional plasmonic fields. This approach is based on meta structures and allows the creation of lenses with an effective chirality that depends on the illumination. The coupling structures are milled into a gold surface and the created SPPs are detected via time-resolved PEEM.

CPP 22.2 Tue 10:45 H8

Advanced optical programming of individual meta-atoms beyond the effective medium approach — •Andreas F. Hessler[1], Ann-Katrin U. Michel[1], Sebastian Meyer[1,2], Julian Pries[1], Yuan Yu[1], Martin Lewin[1], Tobias W. W. Mass[1], Matthias Wuttig[1], Dmitry N. Chigrin[1,2], and Thomas Taubner[1] — [1]Institute of Physics (IA), RWTH Aachen — [2]DWI - Leibniz Institute for Interactive Materials, Aachen

Despite their nanometer thickness, active metasurfaces (MSs) based on phase-change materials (PCMs) enable compact photonic components, offering adjustable functionality for the manipulation of light, such as polarization filtering, lensing and beam steering[1]. Commonly, they feature multiple operation states by switching the whole PCM fully between two states of drastically different optical properties[2]. Intermediate states of the PCM have also been exploited to obtain gradual resonance shifts which are usually uniform over the whole MS and described by effective medium theory. We now demonstrate simultaneous control of size, position and crystallization depth of the switched PCM volume within each meta-atom. By modifying the local optical properties, reflection amplitude and phase can be programmed at the meta-atom scale. This goes beyond previous effective medium concepts and should allow for multiple complex functionalities on the same MS or small adaptive corrections to external aberrations and fabrication errors.
[1] X. Yin et al., Light Sci Appl. 6, e17016 (2017).
[2] M. Wuttig et al., Nat. Photon. 11, 465 (2017).

CPP 22.3 Tue 11:00 H8

A Spin-Optical Nano Device — •Enno Krauss[1], Gary Razinskas[1], Dominik Köck[1], Swen Grossmann[1], and Bert Hecht[1,2] — [1]Nano-Optics and Biophotonics Group, Department of Experimental Physics 5, University of Würzburg, Würzburg, Germany — [2]Wilhelm-Conrad-Röntgen-Center for Complex Material Systems (RCCM), University of Würzburg, Würzburg, Germany

The photon spin is an important resource for quantum information processing as is the electron spin in spintronics. However, for subwavelength confined optical excitations, polarisation as a global property of a mode cannot be defined. Here, we show that any polarisation state of a plane-wave photon can reversibly be mapped to a pseudo-spin embodied by the two fundamental modes of a subwavelength plasmonic two-wire transmission line. We design a device in which this pseudo-spin evolves in a well-defined way throughout the device reminiscent of the evolution of photon polarisation in a birefringent medium and the behaviour of electron spins in the channel of a spin field-effect transistor. The significance of this pseudo spin is enriched by the fact that it is subject to spin-orbit locking. Combined with optically active materials to exert external control over the pseudo-spin precession, our findings could enable spin-optical transistors, i.e. the routing and processing of quantum information with light on a subwavelength scale.

CPP 22.4 Tue 11:15 H8

Magneto-optical thermal Hall effect — •Annika Ott[1], Philippe Ben-Abdallah[2], and Svend-Age Biehs[1] — [1]Institut für Physik, Carl von Ossietzky Universität, D-26111 Oldenburg, Germany — [2]Laboratoire Charles Fabry, UMR 8501, Institut d'Optique, CNRS, Université Paris-Sud 11, 2, Avenue Augustin Fresnel, 91127 Palaiseau Cedex, France

The control of heat flux at the nanoscale by means of external magnetic fields has attracted much attention, recently. It could be shown that the near-field heat transfer between two magneto-optical slabs can be tuned by the external field [1], and unexpected and very interesting effects like the thermal radiative Hall effect, persistent currents, and giant magneto-resistance [2, 3, 4, 5] have been highlighted. Here we discuss the existence of a circular heat flux [6] as the origin of the thermal radiative Hall effect.

References:

1. E. Moncada-Villa, V. Fernandez-Hurtado, F. J. Garcia-Vidal, A. Garcia-Martin, and J. C.Cuevas, Phys. Rev. B 92, 125418 (2015). 2. P. Ben-Abdallah, Phys. Rev. Lett. 116, 084301, (2016). 3. L. Zhu and S. Fan, Phys. Rev. Lett. 117, 134303 (2016). 4. I. Latella and P. Ben-Abdallah, Phys. Rev. Lett. 118, 173902, (2017). 5. R. M. Abraham Ekeroth, P. Ben-Abdallah, J.C. Cuevas and A. Garcia Martin, ACS Photonics, 5, 705-710, (2018). 6. A. Ott, P. Ben-Abdallah, S.-A. Biehs, Physical Review B, 97, 205414 (2018).

CPP 22.5 Tue 11:30 H8

Electroluminescence from transparent graphene nanojunc-

tions — •Christian Ott, Martin Hauck, Sascha Korn, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Staudtstr. 7/Bau A3, D-91058 Erlangen, Germany

Electroluminescence (EL) emitted from metal-metal tunnel junctions has already been observed in STM experiments in the late 80s [1], nevertheless its origin is still under scientific discussion and is usually attributed either to plasmonic modes triggered by the granular nature of current [2] or to blackbody-like radiation of the injected hot electrons [3]. We report on EL emitted from graphene-graphene nanojunctions (GNJ) fabricated from epitaxial graphene on silicon carbide [4]. In stark contrast to STM experiments, GNJs provide a flat, accessible and transparent geometry, allowing an unobscured optical and electron-microscopic access. The observed EL shows a blackbody like spectrum with surprisingly high apparent temperatures well above the damage threshold of the material. Our findings are critically discussed in terms of differences and similarities to other reported experiments (especially STM) to highlight their contribution to the understanding of an elementary process of light-matter interaction.

[1] Schlittler et al., Z. Phys. B. 72, 497 - 501 (1988) [2] Peters et al., PRL 119, 066803 (2017) [3] Downes et al., Applied Physics Letters 81, 7 (2002) [4] Ullmann et al., Nano Letters 14, 5 (2015)

CPP 22.6 Tue 11:45 H8

Towards Niobium Plasmonics for Single Photon Detection — •Ahmed Farag, Monika Ubl, Annika Konzelmann, Mario Hentschel, and Harald Giessen — 4th Physics Institute, Center for Integrated Quantum Science and Technology IQST, and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

With the fast development in single photon based technologies such as quantum computing and quantum cryptography, conventional avalanche photodiodes as single photon detectors are not the optimum tools anymore. They are currently replaced by Superconducting Nanowire Single Photon Detectors (SNSPDs) based on the superconductivity of certain materials. The current challenge with SNSPDs lies in overcoming the trade-off between the detection efficiency and the recovery time. While a large active area will lead to high detection efficiency, the associated high kinetic inductance causes a long recovery time. Plasmonic nanoantennas can play an important role in the absorption enhancement of SNSPDs. These nanostructures provide a high absorption cross section at resonance, significantly larger than their geometric cross section. We present a plasmonic photon detector based on niobium, as one of the common superconductors with low kinetic inductance. Additionally, we are increasing the absorption of our nanostructures even further using the perfect absorber scheme. We fabricated a plasmonic perfect absorber SNSPD, investigated its response to external light at resonance, and proved the plasmonic-based working principle as evidenced by its polarization dependence.

CPP 22.7 Tue 12:00 H8

Probing surface plasmon with phase-shaped electron energy-loss spectroscopy — •Hugo Lourenco-Martins[1], Davy Gérard[2], Jo Verbeeck[3], Giulio Guzzinati[3], and Mathieu Kociak[1] — [1]Laboratoire de Physique des Solides, Université Paris-Saclay, France — [2]L2n, Université de Technologie de Troyes, France — [3]EMAT, University of Antwerp, Belgium

Electron energy loss spectroscopy (EELS) has attracted a large interest due to its efficiency in resolving plasmonic resonance at the nanometer scale. However, it remained intrinsically unable to detect plasmonic phase-related properties. Nevertheless, vortex electron states constitute a perfect candidate to overcome this limitation and measure optical dichroism in an electron microscope [1]. Moreover, it has been recently demonstrated that such probes can be created in an electron microscope by tailoring the phase of the beam [2]. In the present work [3], we developed a semiclassical formalism describing the interaction between an electron probe with an arbitrary phase profile and a plasmonic mode. We showed that the equation ruling this interaction takes the elegant form of a transition matrix between two electron states mediated by the eigenpotentials of the plasmon modes. In this contribution, we will present the theoretical formalism and a wide variety of numerical studies of interactions between different nano-structures and phase-shaped electron probes, with a special emphasis on the experimental feasibility of the proposed geometries. [1] Asenjo-Garcia et al. PRL 113 (2014) [2] Verbeeck et al, Nature 467 (2010) [3] Guzzinati et al., Nature Com. 8 (2017)

CPP 22.8 Tue 12:15 H8

Quantitative phase imaging of plasmonic metasurfaces — •Vlastimil Křápek[1], Petr Dvořák[1], Alexander Fassbender[2], Petr Bouchal[1], Martin Hrtoň[1], Jiří Babocký[1], Filip Ligmajer[1], Radim Chmelík[1], Stefan Linden[2], and Tomáš Šikola[1] — [1]Central European Institute of Technology, Brno University of Technology, Purkyňova 123, 612 00 Brno, Czech Republic — [2]Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany

We report on wide-field quantitative phase imaging of plasmonic metasurfaces by coherence-controlled holographic microscopy [1] and 4th generation quantitative optical microscopy. Both resonant [2] and geometric phase [3,4] are retrieved for various metasurfaces including a lens and a vortex beam plate. Three-dimensional imaging, polarization sensitivity, and sensitivity down to single antenna is demonstrated.
[1] P. Kolman et al., Opt. Express 18, 21990 (2010).
[2] J. Babocký et al., ACS Photonics 4, 1389 (2017).
[3] A. Faßbender et al., APL Photonics 3, 110803 (2018).
[4] P. Bouchal et al., arXiv 1811.01561.

CPP 22.9 Tue 12:30 H8

Influence of laser parameters on spatially periodic heating of metals induced by surface plasmon polaritons — •Pavel N. Terekhin[1,2], Pascal D. Ndione[1], Sebastian T. Weber[1], and Baerbel Rethfeld[1] — [1]Department of Physics and Research Center Optimas, University of Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany — [2]National Research Centre "Kurchatov Institute", Kurchatov Sq. 1, 123182 Moscow, Russia

We present a detailed investigation of periodic heating of metals and periodic structure formation on their surfaces induced by surface plasmon polaritons (SPPs) after irradiation with ultrashort laser pulses. The interference of the incident and the SPPs electromagnetic waves leads to an enhancement of the resulting field and, therefore, a spatial modulation of the deposited laser energy.

Our aim is to show the influence of laser parameters on the formation of surface structures. The two-temperature model (TTM) is used to calculate the evolution of electronic and lattice temperatures. A new source term in the TTM, which takes into account plasmonic subsystem, is derived. The results obtained indicate that the electronic temperature shows the same spatial oscillations as the source term. Further, these oscillations are still present in the lattice temperature when being heated to the melting point. That could cause the formation of the periodic structures on the surface of the solid. Therefore, the developed model allows calculating materials' heating after ultrashort laser irradiation and studying the fundamental mechanisms of laser energy absorption under controlled conditions.

CPP 23: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge III (joint session O/CPP/DS/TT)

Time: Tuesday 10:30–13:00 Location: H9

Topical Talk CPP 23.1 Tue 10:30 H9

Addressing the structure and dynamics of weakly-bonded interfaces — •Mariana Rossi — Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin

Interfaces between different materials constitute the basis of technological devices. Incorporating organic components within different architectures opens the path for creating more versatile interfaces with a wide range of properties at a reduced cost. However, the large conformational space that organic components can explore at finite temperatures and the inherent anharmonicity of their intra and intermolecular interactions brings further challenges to first-principles simulations. In this talk, I will discuss our recent efforts to address these challenges, based on developments within density functional theory an ab initio (path integral) molecular dynamics. I will present strategies for conformational space sampling of organic/inorganic interfaces, discuss the relationship between atomic and electronic structure including the effect of different functionals, present techniques to include anharmonicity in vibrational fingerprints and machine learning tools to calculate these at reduced costs, and our recent methodological developments that allow the inclusion of quantum nuclear effects in high-dimensional systems (especially weakly bonded interfaces) using path integral molecular dynamics.

CPP 23.2 Tue 11:00 H9

Elucidating the Nuclear Quantum Dynamics of Intramolecular Double Hydrogen Transfer in Porphycene — •Yair Litman[1], Jeremy O. Richardson[2], Takashi Kumagai[1], and Mariana Rossi[1] — [1]Fritz Haber Insitute of the Max Planck Society, Berlin, Germany — [2]ETH, Zurich, Switzerland

We address the double hydrogen transfer (DHT) dynamics of the porphycene molecule: A complex paradigmatic system where the making and breaking of H-bonds in a highly anharmonic potential energy surface requires a quantum mechanical treatment not only of the electrons but also of the nuclei[1]. We combine density-functional theory calculations, employing hybrid functionals and van der Waals corrections, with recently proposed and optimized path-integral ring-polymer methods for the calculation of vibrational spectra and reaction rates. Our simulations predict the position and width of the N-H stretching band of porphycene and DHT rates in excellent agreement with experiments, thus confirming our determination of the tunneling pathways and the anharmonic mode couplings that play a role in this reaction. They also provide quantitative information about the usually ignored competition between concerted and stepwise DHT pathways at different temperature. These results show that our theoretical approach can describe hydrogen transfer dynamics in different environments, for example when porphycenes are adsorbed on surfaces in prototype molecular switch architectures[2]. [1] Y. Litman, Richardson, J. O., Kumagai, T., Rossi, M. *arXiv*:1810.05681. [2] T. Kumagai, et al., *J. Chem. Phys.,* **148,** 102330 (2018).

CPP 23.3 Tue 11:15 H9

Interplay of quantum nuclear fluctuations and the electronic structure of the cyclohexane/Rh(111) interface — •Karen Fidanyan and Mariana Rossi — Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, Berlin

Cyclohexane (C_6H_{12}) adsorbed on metal surfaces can participate in catalytic dehydrogenation reactions, which show good potential for hydrogen storage. It has been observed experimentally that C_6H_{12} adsorbed on the Rh(111) surface shows an isotope effect on the work function change and the adsorption energy upon deuteration [1]. The physical origin of this puzzling isotope effect on the electronic structure has not been fully resolved. We employ density-functional theory (PBE functional with van der Waals corrections) and *ab initio* path-integral molecular dynamics at 150 K to characterize the underlying physics of this phenomenon. We perform these simulations almost at classical-nuclei cost by making use of the spatially-localized ring-polymer contraction scheme proposed in Ref. [2]. The harmonic approximation to zero-point-energy in the adsorption energy is not able to capture the isotope effects observed experimentally. We thus include anharmonic corrections through the dynamics and identify the temperature-dependent electronic level broadening and renormalization due to the interaction with phonons in this system.

[1] T. Koitaya and J. Yoshinobu, *Chem. Rec.* **14** 848-856 (2014).

[2] Y. Litman, D. Donadio, M. Ceriotti and M. Rossi, *J. Chem. Phys.* **148** 102320 (2018).

CPP 23.4 Tue 11:30 H9

Quantum-Nuclear Effects in Anharmonic Thermal Transport of Organic Materials — •Hagen-Henrik Kowalski, Mariana Rossi, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

To date, an accurate computational assessment of thermal transport in organic compounds still constitutes a considerable challenge for first principles theory, since the vibrations in such compounds are to a large extent governed by quantum-nuclear (QN) ***and*** strongly anharmonic (SA) effects [1]. Perturbative approaches account for QN, but not for SA effects, whereas Molecular Dynamics (MD) approaches [2] with classical nuclei account for SA, but neglect QN effects. To overcome this limitation, we here present a framework capable of accounting for both QN and SA effects by sampling the vibrational motion via Thermostatted Ring Polymer Molecular Dynamics (TRPMD). The lattice thermal conductivity is assessed through the Green-Kubo formalism and the auto-correlation of the heat flux. To obtain this quantity, we extend the *ab initio* heat-flux definition proposed in Ref. [2] from MD to TRPMD, in order to include QN effects. We critically discuss the approach, its accuracy, and numerical cost for several materials, ranging from toy-models, e.g., solid Argon, to recently discussed organic materials, in which both QN and SA effects are non-negligible.

[1] M. Rossi, P. Gasparotto, M. Ceriotti, *Phys. Rev. Lett.* **117**, 115702, (2016).

[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901, (2017).

CPP 23.5 Tue 11:45 H9

Electronic Conduction in Metal Junctions with Multi-Heme Proteins — •Zdenek Futera[1], Xiuyun Jiang[1], Jan Elsner[2], and Jochen Blumberger[1,3] — [1]Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom — [2]University of Cambridge, Robinson College, Grange Road, Cambridge CB3 9AN, United Kingdom — [3]Institute for Advanced Study, Technische Universität München, Lichtenbergstrasse 2 a, D-85748, Garching, Germany

Multi-heme proteins such as STC or MtrF are membrane proteins facilitating long-range electron transfer (ET) across cell membrane in metal-reducing bacteria. We have used classical molecular dynamics (MD) together with electronic-structure calculations based on density functional theory (DFT) to show that in native environment the conducted electrons are transferred by incoherent hopping between the heme cofactors. However, recent experimental measurements of current-voltage (I-V) curves suggested that the ET mechanism changes to coherent electron tunneling in vacuum when the protein is electronically coupled with metal electrodes. To investigate such conditions, we performed MD simulations in accurate gold/protein interaction force field to identify adsorption of STC and MtrF between two gold electrodes. By large-scale DFT calculations of the whole interfacial structure we identified the conduction channels formed predominantly by delocalized heme iron states. Finally, we apply Landauer formalism to compute I-V curves on STC junction using the DFT electronic states corrected for band alignment and discuss the ET mechanism.

CPP 23.6 Tue 12:00 H9

Elastic and lattice-dynamical properties of titanium-based compounds — •Peter Weber, Pasquale Pavone, and Claudia Draxl — Humboldt-Univeristät zu Berlin, Physics Department and IRIS Adlershof, Germany

Titanium is the basic element of a variety of compounds with very different electronic, mechanical, and thermal properties. While, for instance, the rocksalt crystals TiC and TiN are well known for their hardness, allotropes of TiO_2 show much softer elastic behaviour. In this work we present the results of an *ab-initio* investigation of the elastic and lattice-dynamical properties of these compounds under pressure. The elastic-constant tensor is calculated up to the third order. Pressure effects on the lattice-dynamical properties of these compounds are evaluated in terms of the mode Grüneisen parameter at the Brillouin zone center. The calculations are performed using density-functional theory as implemented in the full-potential all-electron software package `exciting` [1]. Linear and nonlinear elastic constants are obtained using the `ElaStic` tool [2].

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26** (2014) 363202
[2] R. Golesorkhtabar *et al.*, Comp. Phys. Commun. **184** 1861 (2013)

CPP 23.7 Tue 12:15 H9

Understanding the electron transport through NiSi$_2$-Si interfaces — •Florian Fuchs[1,2,3,4], Sibylle Gemming[1,2,3], and Jörg Schuster[2,4] — [1]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]Center for Advancing Electronics Dresden (cfaed), Dresden, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — [4]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Metal-semiconductor interfaces are of huge importance for applications and can be found in various field-effect transistors. We study the interface between NiSi$_2$ and silicon on the basis of density functional theory and the NEGF formalism. Different crystal orientations and strain states are investigated systematically.

We focus on the tunneling phenomena of carriers through the Schottky contact at the interface, which are crucial for the on-current in transistors. The on-current is found to be strongly dependent on strain and orientation. It will be shown that the height of the Schottky barrier determines the tunneling current. However, not all changes in the current can be traced back to the barrier height. The modification of the electronic structure matter as well, which can be modeled based on the effective mass of the tunneling carriers. We have also extracted work functions of the isolated materials which we relate to the extracted Schottky barrier heights. It will be shown that the Schottky-Mott model fails for this material system. Better approaches will be discussed in our contribution.

CPP 23.8 Tue 12:30 H9

Impact of Lattice Screening on Wannier-Mott Excitons — •Claudia Rödl — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Optical properties of materials are most relevant for a large variety of technological applications, ranging from photovoltaics over various spectroscopy techniques to LEDs and displays. In optical spectra, microscopic quantum many-body effects like excitons, i.e. coupled electron-hole-pair excitations, are measurable at a macroscopic scale and crucially determine the materials properties. Hence, a deep understanding of exciton physics constitutes an indispensable driving force for innovation in optics and optoelectronics.

The state-of-the-art parameter-free theoretical description of excitons is based on the Bethe-Salpeter equation of many-body perturbation theory. The present theoretical standard approach takes only the static electronic screening of the electron-hole-pair interaction into account. The coupling of excitons to phonons and, hence, polaronic screening contributions are omitted. However, the exciton-phonon coupling is crucial for the qualitative and quantitative understanding of exciton spectra in materials with strong polaronic effects, such as many technologically highly relevant oxides. We will tackle this problem and explore routes towards the inclusion of the polaronic screening contributions into the Bethe-Salpeter framework. As test systems, we study simple two-atomic bulk semiconductors and insulators.

CPP 23.9 Tue 12:45 H9

Discovering a novel nanometric cubic phase in monochalcogenide semiconductors - Theory meets experiment — •Guy Makov[1,2], Uri Argaman[1], Elad Segev[2], Ran Abutbul[1,2], and Yuval Golan[1,2] — [1]Dept. of Materials, Ben-Gurion University, Beer-Sheva, Israel — [2]Ilse Katz Institute of nanoscience, Ben-Gurion University, Beer-Sheva, Israel

A new nanometric cubic binary phase with a low-symmetry 64-atom cubic structure was recently discovered in tin monosulfide. Subsequently, this phase was synthesized and identified in tin monoselenide and posited to exist in germanium monosulfide and monoselenide based on density functional theory total energy calculations. A series of computational and experimental studies have identified promising optical properties due to the larger bandgap and non-centrosymmetric structure of the crystal. The structure, atomic positions, band gaps and vibrational spectra of these phases were determined by ab-initio density functional calculations and found to be in very good agreement with experimental measurements. The phases were determined to be mechanically stable from ab-initio phonon spectra and energetically close to competing structures such as rhombohedral and orthorhombic. Surface energy calculations indicate that the particles must be stabilized by ligand adsorption. Ligand surface properties are explored to explain the nanocrystal growth mechanisms. This talk will focus on the results of our calculations on surface and bulk properties and their interplay with experimental studies.

CPP 24: Focus: Mechanoresponsive Molecules and Materials - organized by Kerstin Blank and Robert Göstl

Time: Tuesday 10:45–13:00 Location: H14

Invited Talk CPP 24.1 Tue 10:45 H14

Mechanochemical activation of Cu-NHC-complexes : molecular design, force-measurements and application in polymer materials — •Wolfang H Binder[1], Michel Biewend[1], Philipp Michael[1], Martin Beyer[2], and Matthew Sammon[2] — [1]Martin-Luther University Halle-Wittenberg, Institute of Chemistry, Chair of Macromolecular Chemistry — [2]Leopold-Franzens-Universität Innsbruck, Institut für Ionenphysik und Angewandte Physik

Understanding rupture of single chemical bonds is an important aspect in chemistry, physics and biology, as many bonds form and reform reversibly, imparting dynamic properties into a molecule or the material it is embedded into (eg. DNA-replication, protein-assembly). However, rupture of covalent bonds can also be induced by molecular force when acting on a chemical bond, enabling bond breaking by distortion. We here report on a metal-complex designed to be activated by molecular force, transmitted via bound polymer chains acting as molecular handles. We will discuss the chemical nature of the metal-complex acting as a mechanophoric system, followed by considerations to measure the molecular force by AFM. Designed cyclic mechanophores enable to discriminate true disruptive events from purely thermal induced debonding events. The use of molecular networks to efficiently transmit force onto the labile mechanochemical bonds will be discussed in view of force-detection in polymeric materials. References: Chem. Soc. Rev. 2011, 40, 2359; MRC, 2018, 0, 1800376; Angew. Chem., Int. Ed. 2015, 54, 13918; Angew. Chem. Int. Ed. 2015, 54, 2556.

15 min. break

Invited Talk CPP 24.2 Tue 11:30 H14

Mechanoradicals in collagen or: Why playing soccer hurts — •Frauke Gräter[1,2], Christopher Zapp[1,2], Agnieszka Obarska-Kosinski[1], Csaba Daday[1], and Reinhard Kappl[3] — [1]HITS, Heidelberg, Germany — [2]Interdisciplinary Center for Scientific Computing, Heidelberg University, Germany — [3]Medical Center of Saarland, Homburg, Germany

Polymers subjected to mechanical stress - be it a shoe sole or rubber band - generate mechanoradicals by undergoing homolytic bond scission. The existence, nature and mode of action of mechanoradicals formed in protein materials under physiological levels of loading, are fully unknown. I will present our recent results on mechanoradicals in collagen. Electron-paramagnetic resonance (EPR) spectroscopy of stretched rat tail tendon fascicles in conjunction with atomistic Molecular Dynamics simulations of collagen I model fibrils show that the radicals form by bond scission in the direct vicinity of crosslinks along the fiber. Radicals then migrate to the adjacent clusters of aromatic residues where they are stabilized. They finally convert into hydrogen peroxide, a key redox signaling molecule. Our work proposes protein mechanoradicals as a yet undiscovered source of oxidative stress, with potential links to processes such as pain sensation and inflammation. Being exposed to extreme loads, collagen I evolved as a radical sponge, a defense against mechano-oxidative damage.

CPP 24.3 Tue 12:00 H14

Joint experimental and computational design of tunable molecular photoswitches based on Hemithioindigo compounds — •Martin Lea, Barney Lewis, Michael Staniforth, Vasilios Stavros, and Reinhard J. Maurer — Univeristy of Warwick, Coventry, United Kingdom

The ability to reversibly modify the properties of a material in response to external stimuli is fundamental for the design of novel functional materials. Being able to manufacture and control this ability at the molecular level could lead to the realization of the next generation of nanomaterials for sensors and optoelectronics. Achieving an understanding of how chemical modifications can be used to augment or even inhibit switching will enable intuitive component design for the fabrication of tailor-made, light responsive materials and interfaces.

An emerging class of photoswitching molecules are Hemithioindigos (HTIs). HTIs exhibit exciting photoisomerization properties which can be tuned through means of chemical functionalization. Here we present a joint first-principles-based computational and spectroscopic experimental study on the influence functional groups have upon the key design parameters of HTIs that enable the switching capabilities. These design parameters include spectral properties and the thermodynamic stability of the equilibrium compounds, but also parameters that capture the ground - and excited - state landscapes that determine the photodynamics. On the basis of our findings, we propose molecules with a propensity for successful switching in different applications.

CPP 24.4 Tue 12:15 H14

How mechanical properties of coiled coils depend on the oligomerization state: comparing dimers and trimers using molecular dynamics simulations — •Ana Bergues-Pupo, Reinhard Lipowsky, Kerstin Blank, and Ana Vila Verde — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Coiled-coils (CCs) are ubiquitous motifs in many proteins of the cytoskeleton, extracellular matrix and also in bio-engineered materials. The study of their mechanical response is crucial to understand their function and to tune their properties for specific applications. The relationship between CC sequence-structure and mechanics at the molecular level is however not fully understood. Here, we investigate different aspects of CC topology in the mechanical response under shear stress by means of molecular dynamics simulations: we compared a dimer and a trimer CC of similar sequence composition and also look at the effect of amino acids mutations and single helix stability in the mechanical response of the trimer.

The trimeric coiled coil is mechanically more stable than the dimer. The molecular mechanisms of deformation are also different: trimer exhibits irreversible helix unfolding, while unfolding/refolding assisted sliding is observed for the dimer. Interestingly, this increase on stability is almost unaffected by mutations on the hydrophobic and charged amino acids of the trimer. These interactions are known to be determinant for the thermodynamic stability. On the other hand, the mechanical strength of the trimer considerably increases if helical strength is increased such that single helix unfolding is prevented.

Invited Talk CPP 24.5 Tue 12:30 H14

The challenges and opportunities of polymer mechanochemistry — •Roman Boulatov — University of Liverpool, Liverpool, UK

Polymer mechanochemistry is an emerging field at the interface of chemistry, materials science, physics and engineering. It aims at understanding and exploiting unique reactivities of stretched polymer chains. Macromolecules or their segments become stretched in bulk polymers under mechanical loads or when polymer solutions are sonicated or flow rapidly through abrupt contractions. Increasing amount of empirical data suggest that mechanochemical phenomena are widespread wherever polymers are used. In the past decade, empirical mechanochemistry has progressed enormously, from studying fragmentations of commodity polymers by simple backbone homolysis to demonstrations of self-strengthening and stress-reporting materials and mechanochemical cascades using purposefully designed monomers. Progress in developing the conceptual foundation of mechanochemistry has been more limited. I'll discuss this progress and the outstanding challenges facing polymer mechanochemistry.

CPP 25: Poster Session II

Topics: Complex Fluids and Colloids, Micelles and Vesicles (25.1-25.10); Composites and Functional Polymer Hybrids (25.11-25.18); Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods (25.19-25.20); Hydrogels and Microgels (25.21-25.26); Modeling and Simulation of Soft Matter (25.27-25.35); Nanostructures, Nanostructuring and Nanosized Soft Matter (25.36-25.44); Responsive and Adaptive Systems (25.45-25.49); Wetting, Fluidics and Liquids at Interfaces and Surfaces (25.50-25.58).

Time: Tuesday 14:00–16:00 Location: Poster B1

CPP 25.1 Tue 14:00 Poster B1

Thermodiffusion of Binary Halobenzene-n-Alkane Mixtures — •Bastian Pur, Florian Schock, and Werner Köhler — Universität Bayreuth, 95440 Bayreuth, Germany

The Soret effect (thermophoresis) describes a diffusion flux that is driven by a temperature gradient in a multicomponent mixture. For dilute solutions of polymers with large Kuhn segments there is a remarkable universality for the thermophoretic velocity: it depends only on the viscosity η of the solvent. The thermal diffusion coefficient D_T, also known as the thermophoretic mobility, multiplied by the solvent viscosity leads to a constant value ($\eta D_T \approx$ const.). This universality is asymptotically also found for binary mixtures of methylnaphtalene and toluene in n-alkanes. To pursue these observations we have conducted measurements with halobenzene-n-alkane mixtures. The measured mixtures correspond to the series of halobenzenes fluoro-, chloro- and bromobenze mixed with n-alkanes nC_i (i=6,7,8,10,12,14 and 16). By means of a holographic grating technique we have obtained the Fickian diffusion coefficient D, the Soret coefficient S_T and the thermal diffusion coefficient D_T. These results will be compared to the universal asymptotic limit of ηD_T reported for polymer solutions.

CPP 25.2 Tue 14:00 Poster B1

Measurement of transport processes in multicomponent liquids by multi-color techniques — •Marcel Schraml, Pascal Möckel, Felix Sommer, and Werner Köhler — Department of Physics, University of Bayreuth, 95447 Bayreuth

Diffusive flows in a non-isothermal multicomponent fluid are characterized by complex cross-coupling phenomena between all concentration and temperature gradients. Since the number of unknown coefficients increases quadratically with the number of components, such multicomponent systems quickly become intractable, and today's research focuses mainly on ternary mixtures as multicomponent model systems.

Within the ESA/Roscosmos DCMIX program, measurements are performed both under microgravity conditions aboard the International Space Station ISS and in various laboratories on ground. In order to resolve all components, optical multicolor beam deflection and interferometry experiments are typically employed. The most critical step in the data analysis is the transformation from the multicolor refractive index space to the compositions, for which the so-called contrast factor matrix must be inverted. Since this matrix is frequently ill-conditioned, extremely precise measurements of the partial derivatives of the refractive index with respect to the composition variables and the temperature are required.

In our poster we will present the optical multi-color techniques employed both on ground and in space and discuss consistent multicolor measurements of the optical contrast factors.

CPP 25.3 Tue 14:00 Poster B1

Camphor/Succinonitrile – a model system for metal alloys subjectedto a temperature gradient — •Felix Sommer[1], Marcel Schraml[1], Bastian Pur[1], Werner Köhler[1], Gerhard Zimmermann[2], and Laszlo Sturz[2] — [1]Physikalisches Institut, Universität Bayreuth — [2]Access e.V. Aachen

Hypoeutectic Succinonitrile/Camphor alloys serve as model systems for the solidification of binary metal alloys. The development of the solidification patterns strongly depend on the solute transport at the solid-liquid interface, which is often assumed to be diffusional, even in a thermal gradient. Under such nonequilibrium conditions in a thermal gradient, diffusive flows are characterized by complex cross-coupling phenomena between concentration and temperature gradients. As a consequence, the local composition can significantly shift away from its initial concentration, resulting in unexpected solidification patterns. In order to better understand these mechanisms, we have studied diffusion and thermodiffusion of camphor/succinonitrile binary mixtures around the eutectic composition in the liquid phase. We have been able to determine diffusion, thermodiffusion and Soret coefficients by means of optical beam deflection and photon correlation spectroscopy. For the evaluation of the experiments, precise measurements of the optical contrast factors were performed. Our results prove a significant cross coupling between temperature and composition.

CPP 25.4 Tue 14:00 Poster B1

The Soret effect in ternary mixtures of water + ethanol + triethylene glycol of equal mass fractions: ground and microgravity experiments — •Daniel Sommermann[1], Thomas Triller[1], Marcel Schraml[1], Felix Sommer[1], Werner Köhler[1], Estela Lapeira[2], and Mounir M. Bou-Ali[2] — [1]Physikalisches Institut, Universität Bayreuth, Germany — [2]Mechanical and Manufacturing Department, MGEP Mondragon, Spain

Measurements of the Soret and thermodiffusion coefficients of a symmetric ternary mixture with equal mass fractions of water, ethanol, and tri-ethylene glycol have been performed by two-color optical beam deflection and the thermogravitational column technique in the laboratory and under microgravity conditions in the SODI apparatus aboard the ISS. The results from all three experimental techniques agree within the experimental error bars. The agreement with the microgravity results shows that thermosolutal convection could be well controlled in the 2-OBD experiments by a proper orientation of the temperature gradient. Based on the orientation of the confidence ellipsoid, not all coefficients are equally affected by experimental errors. Although there are appreciable uncertainties for water and ethanol, the Soret and the thermodiffusion coefficients of tri-ethylene glycol could be obtained with a good accuracy. We have found that water behaves thermophobic, whereas both ethanol and tri-ethylene glycol are thermophilic with negative Soret coefficients.[1]

[1] T.Triller et al., Eur. Phys. J. E, submitted 2018

CPP 25.5 Tue 14:00 Poster B1

1D capillary collapse and the role of initial fluctuations in Brownian Dynamics and DDFT — •Anja Schreiber, Johannes Bleibel, and Martin Oettel — Institut für angewandte Physik, Universität Tübingen, Tübingen, Germany

We investigate the so–called capillary collapse of colloidal particles trapped a fluid interface in 1D Brownian Dynamics (BD) simulations. Interfacially trapped, micrometer–sized colloidal particles interact via long–ranged capillary attraction. The interaction is formally analogous to screened Newtonian gravity with the capillary length λ as the tuneable screening length. Within intensive studies of the dynamics in 2D[1], it turned out that radially averaged Dynamical Density Functional Theory (DDFT) only captures the dynamics at initial times and largely deviates from simulation results later on. This discrepancy has been traced to the role of an initially averaged configuration in DDFT[2]. In BD, simulation runs are averaged over initial conditions and noise. The long–ranged potential and initial density fluctuations allow for an early clustering of particles prior to a global, collective collapse similar to a self gravitating fluid. This clustering remains present through most stages of the evolution and renders averaged density profiles, which deviate largely from DDFT. Since the clustering process is much more restricted in 1D, we use 1D simulations in order to shed light on the precise role of initial fluctuations in the averaging process and subsequent dynamics both in BD simulations and DDFT.

[1] Bleibel, Domínguez, Oettel, Dietrich, Soft Matter 10, 4091 (2014).

[2] Bleibel, Domínguez, Oettel, JPCM 28, 244021 (2016).

CPP 25.6 Tue 14:00 Poster B1

Role of pH in Micro-Swimming — •Nadir Möller and Thomas Palberg — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 7, 55128 Mainz, Germany

Modular micro-swimmers are self-assembled systems of colloids that are able to directionally traverse in a low Reynolds number environment after assemlby. In our modular micro-swimmer, a settled ion exchange (IEX) sphere exchanges residual Na+ ions for H+ and thus generates a pH-gradient. This gradient in turn induces a diffusion-electric field which drives an electro-osmotic solvent flow along the substrate. The flow assembles dispersed cargo spheres, which, once assembled break the flow symmetry and set the formed complex in motion. While a comprehensive characterisation of swimmer trajectories, speeds and stability as a function of experimental boundary conditions has been performed, and a theoretical model has been developed, the key input of modelling, i.e. the pH gradients, are available only in approximations. To gain insight of the influence the pH has on the particles motions, we utilize a home-built setup for pH-micro-photometry. This method can be employed in a variety of other systems for characterization of microfluidic and chemical attributes of electro-osmotic-driven particles.

CPP 25.7 Tue 14:00 Poster B1

Competing nucleation and fractionation in hard sphere crystals — •Nicole Schaertl[1], Jennifer Wenzl[1], Thomas Palberg[1], and Eckhard Bartsch[2] — [1]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [2]Institute of Physical Chemistry, Albert Ludwigs University, Freiburg, Germany

Fluid to crystal first order phase transition of monodisperse hard spheres (HS) upon increasing volume fraction was predicted in the 1950s and later confirmed experimentally on sterically stabilized HS approximants [1]. In particle synthesis, size polydispersity is unavoidable. According to theory, a polydisperse fluid should yield coexisting solid phases upon compression [2]. Despite the general anticipation towards fractionation in HS systems, no direct observation has been reported so far. We decided to focus on PS microgel particles with 6% polydispersity in a good solvent. Sufficiently steep steric repulsion for HS-like behavior is obtained at high degree of crosslinking. Recent studies have shown that this colloidal system is less prone to jamming effects than other common HS approximants [3]. This makes this systems particularly interesting for crystallization studies. Time resolved static light scattering revealed several series of well indexable Bragg reflexes shortly after shear melting and re-solidification. This demonstrates the existence of crystals with same fcc structure but different lattice constants. During ripening stage the number of identifiable fractions slowly reduces from half a dozen to three. [1] Pusey, van Megen, Nature 320, 340 (1986) [2] Fasolo, Sollich, Phys. Rev. Lett. 91, 068301 (2003) [3] Schaertl et al., Soft Matter, 14, 5130 (2018)

CPP 25.8 Tue 14:00 Poster B1

Dynamic susceptibility of a cluster interacting superparamagnetic particles in an oscillating magnetic field — •Vladimir Zverev and Alexandr Ambarov — Ural Federal University, Ekaterinburg, Russia

At the present moment several methods for reconstructing the spatial distribution of magnetic particles are being developed. Most of them are based on measurements of the dynamic susceptibility and an ensemble of magnetic nanoparticles is used as a sensitive element. Multicore magnetic nanoparticles allow an increase the temporal resolution and improves the signal-to-noise ratio. In this work we investigate dynamic response of a single cluster of an ensemble of interacting ferroparticles that are formed multicore magnetic particle. It is assumed that the relaxation of the magnetic moments occurs due to Neel mechanism. Dynamic response of a cluster of single-domain particles in a viscous carrier are determined from the solution of the Fokker-Planck equation. The modified mean-field approach of first-order is used to take into account the dipole-dipole interaction. The time dependence of the magnetization is calculated to determine effective magnetic moment and relaxation time.

CPP 25.9 Tue 14:00 Poster B1

Colloidal particle sizing using various techniques — •Kathrin Eitel and Hans-Joachim Schöpe — Institut für Angewandte Physik, Tübingen

Nanoscience and nanotechnology are playing key roles in different scientific disciplines and its importance increased significantly over the last years. Particle size analysis is of essential importance in research and development as well as in industrial production. Different techniques are used for particle sizing, all given optimal results in a certain particle size range. In dispersions of nano- to micrometer-sized particles, DLS is commonly used. DDM might be a more exact alternative method for particle sizing. In this work, we compared DDM with the established methods such as DLS and SLS working out their advantages and disadvantages.

Keywords: colloids, SLS, DLS, and DDM.

CPP 25.10 Tue 14:00 Poster B1

Pressure-induced phase transition 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 thermal energy storage or medical chemistry. Silica nanoparticles in aqueous solution show a repulsive Coulomb interaction. By adding non-adsorbing polymers (e.g. polyethylene glycol), the total particle-particle interaction can become more attractive. With increasing polymer concentration, the system undergoes a phase transition from the homogenous phase into a liquid-liquid phase separated phase (LLPS). If the system is exposed to high pressure the system switches back into the homogenous phase. In this work, light transmission and small-angle X-ray scattering measurements on systems, containing 1 wt.% silica nanoparticles and various molecular weight and concentration of PEG, were performed to understand of the phase transition on a microscopic level. By combining these techniques, we were able to determine a pressure-dependent phase diagram, and obtained information about typical distances between the nanoparticles in the LLPS phase. The measurements showed that the transition pressure strongly depends on concentration and the size ratio between the polymers and the nanoparticles.

CPP 25.11 Tue 14:00 Poster B1

Polymers for lithium ion batteries - investigating composite electrodes — •Cristian Telescu, Simon J. Schaper, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany.

With the development of new technologies the demand for reliable, cheap and long life batteries with high specific energy and high efficiency is constantly increasing. Therefore, a significant effort is devoted to the improvement of battery performance. The lithium-ion polymer battery is a prospective candidate for powering the new generation of electrical devices and vehicles due to outstanding advantages as low weight, high negative potential and high specific capacity. These features are of critical significance for the automotive and electronics industries. Improving materials, composition, and interfaces is still necessary to exploit the possibilities of polymer based lithium-ion batteries. In this work, a study of polymer composite cathodes with lithium iron phosphate (LFP) and lithium nickel cadmium aluminum oxide (NCA) as active materials is presented and the key performance results are provided.

CPP 25.12 Tue 14:00 Poster B1

Influencing the properties of fullerene-free bulk heterojunction blends for photovoltaic applications — •Amir Kotobi[1], Sebastian Grott[1], Claudia Ott[2], Tom Nilges[2], and Peter Müller-Buschbaum[1] — [1]1TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]2 TU München, Department Chemie, LS innovative Materialien, Lichtenbergstraße 4, 85748 Garching

Over the past decades, organic electronics have attracted increased focus in the field of research. Especially organic solar cells received a high attention, due to their advantages, such as the tuneability of photo-active properties, the possibility to be produced at low-cost, the flexibility and the light-weight, compared to commonly-used inorganic based solar cells. Recently, the most widely investigated bulk heterojunction donor-acceptor system of P3HT:PCBM was doped with iron oxide nanoparticles, resulting in an increase of efficiency. Based on this approach, we investigate the effect of doping photoactive layers consisting of the low-bandgap polymer PBDB-T and the non-fullerene acceptor ITIC with SnIP nanoparticles We study the influence of different nanoparticle concentrations on current-density voltage characteristics and the absorbance. These optoelectronic properties are related to structure information obtained via advanced scattering techniques in order to optimize the device performance.

CPP 25.13 Tue 14:00 Poster B1

Synthesis of Well-Controlled Titania Hollow Spheres — •Anna Lechner and Markus Retsch — University of Bayreuth, Bayreuth, Germany

Over the past few decades, the interest in titania based materials increased enormously because of its strong oxidative potential and photocatalytic activity.

The controlled synthesis of monodisperse and well-defined titania particles on the mesoscale still poses a challenge. In particular core-shell architectures and hollow spheres are interesting titania morphologies owing to their hierarchical architecture controlled by a large diameter and thin shell. In contrast to the synthesis of silica hollow spheres, the synthesis of titania hollow spheres is more challenging because of the highly reactive precursors.

This contribution presents the three steps of a controlled and scalable synthesis of titania hollow spheres of various sizes. First, the synthesis of polystyrene particles via dispersion polymerization is explained. Here, several parameters for the adjustment of the particle size are discussed. Furthermore, the synthesis of smooth titania shells of defined thicknesses is presented following a simple precursor condensation strategy. Finally, the template core removal can compromise the integrity of the titania shell. We assess strategies to retain the structural control to yield monodisperse titania hollow spheres.

We will also provide an outlook of the exciting properties of such hierarchically structured porous titania materials with respect to their optical and thermal transport properties.

CPP 25.14 Tue 14:00 Poster B1

Thermo-mechanical behavior of silver-filled thermoplastic polymers — •Amira Baccari and Peter Müller-Buschbaum — TU München, Physik Department, LS Funktionelle Materialien, 85748 Garching, Germany

Filled thermosetting and thermoplastic polymers are used for silver-filled, electrically conductive adhesives in the printed circuit board industry. These are a type of glue containing usually 80% of a conductive material and 20% of a polymer matrix that has the necessary mechanical and thermal properties. The produced electronic devices need to pass several thermo-mechanical tests using dynamic mechanical analysis and thermal mechanical analysis (DMA and TMA) techniques in order to get a good expectancy of the lifetime performance and behavior of the products. Companies concerned with the manufacturing of electronics want to use experiments and simulation for assessing a new adhesive based on a thermoplastic polymer matrix (instead of the usual epoxy-based composite adhesive). Thermo-mechanical material models of polymers are essential for obtaining meaningful results from thermo-mechanical simulation. The electronics packaging community has an acceptable understanding of the thermo-mechanical behavior of thermosetting epoxy polymers, but not yet of silver-filled thermoplastic polymer matrices, which will be focused in this work.

CPP 25.15 Tue 14:00 Poster B1

Polybutadiene in Alumina nanopores — •Lama Tannoury — Institute of Physics, Martin Luther University, Halle (Saale), Germany

Several studies concerning 1,4-polyutadiene (PBD) confined between graphite walls have been performed perviously. They have shown that the polymer melts experience, at close distances to the confining walls, a variation in both monomer and chain density. Furthermore, that layer also experiences a change in dynamics incorporated in the slowing down of and an extra process of relaxation. These studies are essential to the comprehension of composite materials made of polymer matrices and inorganic filler particles such as rubber tires. The latter is a composite material filled with nanoparticles. However, since previous research on PBD melts permeated by nano-sized fillers could not reach relaxation time scales accessible by Molecular Dynamics (MD) simulations, we attempt to study a chemically realistic model of a PBD melt inside alumina and silica pores using the GROMACS package. We aim to enhance our view concerning bulk relaxation processes and any modifications they experience due to confinement.

CPP 25.16 Tue 14:00 Poster B1

Magnetic Nanoparticle / Polymer Brush Composites: The Effect of pH and Concentration on Particle Adsorption — •Philipp Ritzert, Dikran Boyaciyan, and Regine v Klitzing — Soft Matter at Interfaces, Institut für Festkörperphysik, TU Darmstadt

Polymer chains, which are end-grafted chemically to a substrate are referred as polymer brushes and have attracted a growing interest in the field of surface coating over the last few decades due to their high mechanical and chemical stability. Based on the functional group of the monomer unit, it may exhibit sensitivity to external stimuli, such as temperature, pH or solvent (1). Polymer brushes can bind different kinds of material with a high selectivity, depending on the available functional groups. Recent studies demonstrated the incorporation of nanoparticles into different kinds of polymer brushes (1; 2; 3). In the case of gold nanoparticles (AuNPs), the uptake induced novel optical properties, due to the Surface Plasmon Resonance of the AuNPs (3).

The present work demonstrated the successful immobilization of magnetic nanoparticles (MNPs) on Poly(N-isopropylacrylamide) (PNIPAM) brushes. The pH-sensitive citrate capping of the MNPs stabilizes the MNPs in the neutral to basic pH regime and simultaneously binds to the PNIPAM brush via H-bonding. The goal of this work is to characterize the adsorption of MNP on PNIPAM brushes by changing the pH value and concentration of the MNP suspension.

1. S. Christau, et al. Macromolecules. 2017, 50, pp. 7333-7343.
2. D. Boyaciyan, et al. SoftMatter. 2018, 14, pp. 4029-4039.
3. S. Christau, et al. Polymers. 2014, 6, pp. 1877-1896.

CPP 25.17 Tue 14:00 Poster B1

Thermoelectric Characterization of Polymer Composite Thin Films — •Marie Siegert[1], Alexander Steeger[2], 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, organic thin films have become of interest for thermoelectric applications as a low-cost, sustainable alternative to inorganic semiconductors. To achieve a high thermoelectric figure of merit $zT = \sigma S^2 T/\kappa$, which is a measure for the efficiency of converting waste heat into electricity, the thermal conductivity κ of the thin film needs to be minimized, while maximizing its electrical conductivity σ. Polymer thin films, which can be prepared by solution processing at large scales, exhibit sufficiently low thermal conductivities, but lack high electrical conductivity as a result of their inherent disorder. In contrast, crystalline organic metals, requesting high efforts on their preparation, show superior charge carrier transport characterized by a metallic conductivity behavior over a wide temperature range [1]. Here we report on the combination of the two material approaches by preparing composite thin films of the well studied polymer PEDOT:PSS blended with crystallites of the low-dimensional molecular metal TTT_2I_3. First results on the electrical and thermal properties of these polymer-molecular metal composites will be presented and evaluated with respect to their application potential in thin film based thermoelectric generators.

[1] F. Huewe, A. Steeger, et al., Adv. Mat. 29 (2017) 1605682

CPP 25.18 Tue 14:00 Poster B1

Characterization of interfaces in coextruded polypropylene-based multilayer structures via confocal Raman spectroscopy — •Claudia Leimhofer[1], Sabine Hild[1], and Elias Mayrhofer[2] — [1]Institute of Polymer Science, Johannes Kepler University, Linz, Austria — [2]Institute of Polymer Extrusion and Compounding, Johannes Kepler University, Linz, Austria

Co-extrusion of polymers is a powerful tool to produce multilayer composites that combine properties which cannot be achieved by pure substances alone. The strength of the total composite is determined by the adhesion between the adjacent layers. The polyolefines used in industrial applications often are non-polar and show low surface free energy which impairs the overall adhesion. Different adhesion mechanisms for polymers were proposed in the literature. One widely accepted model is based on interdiffusion of the materials and the formation of an interface layer. The aim of the study is to characterize the interdiffusion layers of a co-extruded polypropylene-based composite by confocal Raman spectroscopy. With Raman spectroscopy, the chemical composition of the substances in the bulk layers as well as at the interface can be determined. In the characterized seven-layered systems, a polyethylene- and vinyl alcohol-based barrier layer is combined with a maleic acid grafted polypropylene adhesive, pure polypropylene and a regrind material. The different layers can be clearly differentiated, and the presence of interface layers with spectral properties deviating from the pure substances can be observed.

CPP 25.19 Tue 14:00 Poster B1

Protein dynamics of a thermophile photosystem — •Dominik Schwaiger[1], Maksym Golub[2], Ina Seuffert[3], Athina Zouni[3], Wiebke Lohstroh[4], Peter Müller-Buschbaum[1], and Jörg Pieper[2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Institute of Physics, University of Tartu, Tartu, Estonia — [3]Institute of Biology, Humboldt-Universität zu Berlin, Berlin, Germany — [4]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Garching, Germany

Photosynthesis is the key mechanism in utilization of solar radiation for living organisms and thus provides the base for most food chains and all fossil fuels. The functionality of photosynthetic proteins is - in part- critically influenced by dynamics on a timescale of pico- to milliseconds and on sub-nanometer length scale. The neutron time of flight spectrometer TOFTOF at MLZ-Garching is well suited to study such dynamics, and we currently develop a laser pump setup for TOFTOF allowing us to trigger photoreactions and subsequently probe the dynamics of specific functional states with neutrons. In a first step towards time-resolved measurements, static quasielastic neutron scattering (QENS) experiments were performed on photosystem II (PSII) complexes of the thermophile bacterium thermococcus elongatus, whose protein dynamics is expected to play a pivotal role in thermal adaptation. Using QENS, we have directly investigated PS II protein dynamics on the picosecond timescale in a range from 200 K to 340 K. The results suggest a shift of the onset of protein dynamics towards higher temperatures in thermophile PSII.

CPP 25.20 Tue 14:00 Poster B1

NMR investigations of microfluidics using stripline geometry — •Raoul Nitzsche, Benjamin Kresse, Alexei F. Privalov, and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstr. 6, 64289, Darmstadt, Germany

NMR spectroscopy with microfluidic devices puts high requirements on the probeheads sensitivity. Due to small sample volumes in the μl range, common high frequency (HF) coils of typically 5 to 10 mm cannot be completely filled. A solution to this problem is the stripline, a component commonly used in HF-technique. A flat wire instead of a coil produces the RF pulse in the NMR experiment and detects the signal. This design allows a high filling factor and a homogeneous RF field for signal enhancement and, thus, also a high time resolution. It enables a lab-on-a-chip implementation which is a simple and effective design to examine small amounts of liquids. The stripline is successfully implemented in NMR spectroscopy using microchannels by the Kentgens group [1]. Our test experiments revealed an increased signal-to-noise ratio and a good spectral resolution, as required to distinguish different molecular species with sufficient time resolution. Our goal is to follow the mixing process of two liquids by recording images in a static field gradient spectrometer. For this purpose, we implemented a Y-shaped microfluidic device in a stripline to control the mixing. This design enables the possibility to monitor chemical reactions in a standard cryomagnet.

[1] P.J.M. van Bentum et al., J. Mag. Res., 189 (2007) 104-113

CPP 25.21 Tue 14:00 Poster B1

Mussel-inspired hydrogels with adhesive potential and mechanical robustness — •Sandra Forg and Regine von Klitzing — Technische Universität Darmstadt, Alarich-Weiss-Straße 10, D-64287 Darmstadt

Polymer hydrogels offer unique properties. Especially their responsiveness to external stimuli including pH and temperature provides a huge potential for various technological applications. Combining this stimuli-responsiveness with adhesive attributes would be of use for tissue engineering or medical purposes. Therefore, hydrogels inspired by marine organisms such as mussels have recently become highly attractive. Mussels can strongly adhere to other substrates even in wet conditions, which is mainly determined by the protein 3,4-dihydroxyphenyl-L-alanine (DOPA). This DOPA-group can easily be incorporated into the hydrogel structure. However, most of these hydrogels are mechanically weak and / or possess a low elastic modulus, which remarkably limits their use in in vivo environments.

In this work, temperature-responsive poly(N-isopropylacrylamide) (PNIPAM) microgels are synthesized. They are modified with DOPA to obtain adhesive properties. Their charge is varied by copolymerisation with the anionic monomer acrylic acid (AA). Moreover, their size and cross-linker content can be tuned. Their properties are studied by DLS and Zetasizer measurements. Afterwards, thin films of these DOPA-modified microgels are produced by spin-coating. They are analysed by static and dynamic indentation measurements to get an insight into the mechanical and rheological properties of thin films.

CPP 25.22 Tue 14:00 Poster B1

Investigation of Non-Equilibrium Actuation Dynamics of Mi-

crogel Disks — •Niklas O. Junker[1], Jonas Staudenmeir[1], Marcel van Dongen[2], Sebastian Meyer[1], Dmitry N. Chigrin[1,2], Ahmed Mourran[2], Martin Möller[2], and Gero von Plessen[1] — [1]Institute of Physics (IA), RWTH Aachen, Germany — [2]DWI - Leibniz Institute for Interactive Materials, Aachen, Germany

Microgels are cross-linked polymer networks of micrometer or submicrometer dimensions. Suspended in a solvent, they can undergo large and fast volume changes in response to variations of external parameters (temperature, pH, etc.). In the present work, microgel disks made of poly(N-isopropylacrylamide) (PNIPAm) homogeneously loaded with gold nanorods have been investigated in water. Nonequilibrium actuation dynamics triggered by rapid heating and cooling is studied. The microgels are found to swell with decreasing temperature much faster than they shrink with increasing temperature. This behavior is systematically studied for different heating rates (up to 150°C/min for conventional heating and up to approximately 1°C/ms for photothermal heating, in which the gold nanorods are used as fast and efficient photoabsorbers and local heaters). Experimental and simulation results are compared for both cases.

CPP 25.23 Tue 14:00 Poster B1

Co-nonsolvency induced self-organization of thermo-responsive block copolymers in thin films — •Christina Geiger[1], Cristiane Henschel[2], André Laschewsky[2], Christine M. Papadakis[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Universität Potsdam, Institut für Chemie, Angewandte Polymerchemie, 14476 Potsdam — [3]TU München, Physik-Department, Physik weicher Materie, 85748 Garching

PMMA-*b*-PNIPAM and PMMA-*b*-PNIPMAM in aqueous solution undergo a reversible shell collapse transition at the lower critical solution temperature (LCST), which can be moderated by gradually introducing organic solvents. In thin film configuration, this co-nonsolvency behavior makes them promising materials for vapor-sensitive nanosensors and actuators. We prepare and examine thin films exhibiting various block ratios and subsequently perform swelling experiments in mixed vapor atmospheres. Morphological changes, as well as the kinetics of individual solvent and cosolvent diffusion into the films, concentration gradients and the development of thickness and refractive index are investigated with a focus on white light interferometry and *in-situ* TOF neutron reflectometry experiments.

CPP 25.24 Tue 14:00 Poster B1

Metallo-polymers and -gels based on photosensitive ruthenium(II) complexes and polyethylene glycol — •Leonhard Buchriegler[1], Sabrina Theis[2], Ian Teasdale[3], Sabine Hild[1], and Uwe Monkowius[4] — [1]Institute of Polymer Science, Johannes Kepler University Linz, Austria — [2]Institute of Inorganic Chemistry, Johannes Kepler University Linz, Austria — [3]Institute of Polymer Chemistry, Johannes Kepler University Linz, Austria — [4]Linz School of Education, Johannes Kepler University Linz, Austria

The interest in photo-cleavable polymers has increased significantly due to their broad range of potential applications. The complex $[\mathrm{Ru(II)(bpy)_2(4\text{-}AMP)_2}]^{2+}$ (bpy = 2,2'-bipyridine, 4-AMP = 4-(aminomethyl)pyridine) can be used to generate light-sensitive polyurea supramolecular organogels. This complex has a high photocleavage quantum yield and high storage stability in solution in the dark as well as in neat form. In this contribution, we present a light-sensitive organogel which is composed of the Ru-complex and an 8-arm polyethylene glycol (PEG). The gel is prepared via reaction between amine functions of the Ru-complex and the terminal modified polyethylene glycol forming a crosslinked polyurethane with both 4-(aminomethyl)pyridine ligands connecting two PEG-arms. Irreversible de-gelation occurs within minutes upon irradiation with visible light ($\lambda > 395$ nm), i.e. the Ru-bound pyridine is replaced by a solvent molecule, here acetonitrile. The synthesis and photocleavage-process were investigated by ^{1}H-NMR spectroscopy, mass spectrometry and UV/Vis-spectroscopy.

CPP 25.25 Tue 14:00 Poster B1

Microgel of different topologies: computational study of their properties — •Elena Minina[1,2], Pedro Sanchez[1,2], Christos Likos[1], and Sofia Kantorovich[1,2] — [1]University of Vienna, Vienna, Austria — [2]Ural Federal University, Ekaterinburg, Russia

Nano/microgels are colloidal spherical particles consisting of polymer network. These particles show a fascinating swelling response to external stimuli and therefore are very promising materials in food industry and medicine including drug delivery applications. Due to advances in microgel synthesis, resulting polymer network of nano/microgels can be of different topologies: homogeneous and core-shell topologies. We developed computational coarse-grained models for studying nano/microgels of both topologies. The models are aimed at reproducing microgels synthesized inside a droplet. The main feature of these models is that the resulting polymer network has a random mesh size and its topology depends on the size of the confining sphere where the crosslinking process takes place. We study the structural and swelling properties of the modeled nano/microgels under different solvent conditions. We also include electrostatic interactions to reveal how their influence on the microgel properties.

CPP 25.26 Tue 14:00 Poster B1

Suspensions of magnetic microgels — •Ivan Novikau[1], Elena Minina[1,2], and Sofia Kantorovich[1,2] — [1]University of Vienna — [2]Ural Federal University

Microgels have gained a lot of attention due to their ability to swell and shrink as a response to their external environment [1]. The presence of magnetic particles inside the microgels offers an additional mechanism to control their properties by means of applied magnetic fields.

Study of a single microgel with magnetic particles showed that the magnetic susceptibility of these object strongly depends on the rigidity of the matrix and on the content of magnetic particles [2].

Here, is investigate a suspension of magnetic microgels by means of molecular dynamics computer simulations in order to elucidate possible microgel self-assembly scenarios. Each microgel is initially modeled as bead-spring polymer chains randomly cross-linked into a polymer network. Magnetic particles are randomly incorporated into this network.

Both dilute and relatively dense suspensions of microgels are considered with dipolar interactions in order to observe the self-assembly and figure out which factors are crucial for this process in the zero field case.

[1] A. Fernandez-Nieves, H. M. Wyss, J. Mattsson, and D. A. Weitz. Microgel Suspensions: Fundamentals and Applications. 2011.

[2] E.S. Minina, P.A. Sanchez, C.N. Likos and S.S. Kantorovich, JMMM 459, 226 (2018).

CPP 25.27 Tue 14:00 Poster B1

Computational study of multi-step catalysis in fibrous membranes — •Gabriel Sitaru and Stephan Gekle — University of Bayreuth, Germany

Multi-step catalytic reactions using incompatible catalysts in a one-pot are notoriously difficult to realize in technical settings. In this work, we investigate the potential of fibrous membranes as catalyst carriers by analysing the interplay of three different time scales: advection, diffusion and reaction.

The time-dependent concentration profiles throughout the reactor are computed using a Lattice-Boltzmann based solver for both the advection-diffusion and the Navier-Stokes equations. Using this model it is possible to study various parameters such as flow velocity or different geometries in order to maximize the reaction efficiency.

CPP 25.28 Tue 14:00 Poster B1

Prediction of polymeric nano-structures via machine learning — •Lucia Wesenberg and Ludwig Schneider — Institute for Theoretical Physics, University Göttingen, Germany

The significant length and times scales of the self-assembly of copolymers pose a challenge to particle-based polymer simulation. One possible speed-up strategy consists of using the chemical potential of a non-equilibrium morphology to predict the time evolution. The calculation of the chemical potential by particle-based simulation, however, can take up a vast amount of time, and here we explore the use of machine learning to predict the chemical potential. Machine learning has gained importance due to the introduction of deep neural networks. These enable an efficient implementation of non-linear relations.

Here, we employ this technique to calculate the chemical potential of copolymers in the lamellar phase. Data from different models enable us to tackle the particular interactions separately. First, with data from the Swift-Hohenberg model, we implement the short-range interactions in the neuronal network. Then, we amend the architecture of the network to cover long-range interactions. These are trained using data obtained from the Otha-Kawasaki model. Additionally, a network structure independent of the size of the input data is desirable.

CPP 25.29 Tue 14:00 Poster B1

Machine learning to predict three-body contributions in coarse-graining — •René Scheid, Christoph Scherer, Denis Andrienko, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Coarse-graining (CG) is a method to systematically reduce the degrees of freedom of a given system. Projecting the fine-grained system into a space with lower degrees of freedom leads to higher order interaction terms which are not considered in most CG models. We employ Kernel-based Machine learning (ML) to predict CG contributions based on decomposed CG energies and forces of atomistic simulations. The ML scheme is implemented in the VOTCA-CSG toolkit. First, we show that the ML scheme can recover two-body CG force fields generated by standard force-matching. This demonstrates that the approach is suitable to complement and expand standard force-matched models. Furthermore, we examine the expansion to three-body contributions. Decomposing the CG atomistic interactions into two- and three-body terms, the residual three-body potentials could be used to improve existing two-body models. The approach is illustrated on a Lennard-Jones liquid as test system, liquid water, and liquid methanol.

CPP 25.30 Tue 14:00 Poster B1

Application of data mining techniques in soft matter systems — •Arghya Dutta[1], Luca M. Ghiringhelli[2], Jilles Vreeken[3], and Tristan Bereau[1] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin-Dahlem, Germany — [3]Max Planck Institute for Informatics and Saarland University, Saarland Informatics Campus, Saarbrucken, Germany

Data mining is the method for finding patterns in datasets using techniques borrowed from machine learning and statistics. It is particularly useful when the patterns we are looking for become too intricate to be amenable to a simple physical modelling. I will present results from our ongoing study which show how data mining, particularly text mining and subgroup discovery, can help us in finding patterns, and thus making predictions, in both experimental and computational studies of complex soft matter systems.

CPP 25.31 Tue 14:00 Poster B1

Phase Stability Simulation of Copper Chalkogenide Nanoparticles From First Principles — •Alkit Beqiraj, Ahed Abbousie, Andreas Taubert, and Thomnas Körzdörfer — Uni Potsdam, Am Neuen Palais 10, 14469 Potsdam

Being p-type semiconductors, CuS based nanoparticles demonstrate a large variety of potential applications in optoelectronic devices or energy technology. F.i. CuS nanoparticles can be used as an efficient hole collection layer in an organic solar cell. The CuSx nanoparticles can be synthesized at room temperature using an ionic liquid precursor. This synthesis, however, is very challenging, since even minor variation of the synthesis conditions can change the bias of the reaction, leading to the unexpected precipitation and phase transformation of different oxidative species of copper sulfides. Especially one polymorph of covellite (CuS), i.e., the semiconductor digenit (Cu1.8S), is of particular interest, as it is a frequently encountered byproduct of the synthesis. In order to understand the phase transformation, the chemical parameters, and the nature of the synthesis we carried out DFT calculations. To predict phase stability, vibrational contributions to the free energy were calculated within the harmonic supercell approach. From these calculations, we predict ab initio thermodynamic alloy phase diagrams. From these results, it is possible to analyze which parameters influence the phase evolution of digenit and covellite. Overall, our theoretical results are in a good agreement with the experimental observations and, thus, can be used to intentionally manipulate the experimental conditions in favor of the desired polymorph.

CPP 25.32 Tue 14:00 Poster B1

DFT calculations of K-edge X-ray adsorption spectra for organic molecules — •Rolf Würdemann[1], Julia Melke[1], Anna Fischer[1], and Michael Walter[2] — [1]Freiburger Materialforschungszentrum, Freiburg, Germany — [2]Freiburger Zentrum für interaktive Werkstoffe und bioinspirierte Technologien, Freiburg, Germany

X-ray adsorption spectroscopy (XAS) is an element specific local probe used for the analysis of materials. To compare and interpret these spectra ab initio calculations of XAS spectra can be performed for molecules in given geometries. This can be used to distinguish between different isomers and gain a deeper understanding of the bonding situation.

A common way to calculate XAS spectra by DFT is the utilization of a transition state potential (DFT-TP). In this approach an energetic offset correcting the approximate nature of the used functional has to be applied. To calculate this offset, one has to match the energetic value of the first calculated excitation to experiment. A similar problem in matching energy scales is also known from X-ray photolectron spectroscopy (XPS). Walter et al.[WMP16] have shown, that the offset needed in XPS is nearly constant in respect to the element under consideration and its value can be obtained empirically from experimental data.

In our contribution we extend the approach from Walter et al. to the calculation of XAS spectra and compare our results to experiment.

[WMP16] M. Walter et al., Phys. Rev. B 94 (4), 041112, 2016

CPP 25.33 Tue 14:00 Poster B1

Clarifying the role of 3-body correlations for determining optimal coarse-grained pair potentials — •Svenja Woerner, Kurt Kremer, Tristan Bereau, and Joseph F. Rudzinski — Max Planck Institute for Polymer Research, Mainz, Germany

Structure-based coarse-graining methods often determine optimal pair potentials for reproducing a given set of radial distribution functions. These procedures treat many-body correlations that arise in the condensed phase in various ways. Direct Boltzmann inversion, for example, assumes there are no correlations present in the system, resulting in potentials that tend to overcompensate for the missing correlations. Force matching, on the other hand, uses 3-body correlations from an underlying atomistic model to determine the optimal potentials. This can also result in inadequate potentials, since the coarse-grained model is often incapable of precisely reproducing the atomistic correlations. In this work, we apply the generalized-Yvon-Born-Green integral equation framework to explore the interplay between 2- and 3-body contributions to the pair mean force in coarse-grained models of liquids. As a model system, we consider a one-site per molecule representation for liquid water with isotropic pair interactions. Prominent tetrahedral packing generates 3-body correlations that cannot be reproduced by the coarse-grained model. Our analysis suggests an approach for directly modifying the atomistic 3-body correlations to more accurately reflect the correlations generated by the coarse-grained models.

CPP 25.34 Tue 14:00 Poster B1

Quantifying the reduction of chemical compound space due to coarse-graining — •Kiran Kanekal, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Increasing the efficiency of materials design and discovery remains a significant challenge, especially given the prohibitively large size of chemical compound space. In addition to reducing computational expense, use of a chemically transferable coarse-grained 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, we previously showed that over 400,000 molecules could be mapped to 119 Martini representations, demonstrating a drastic reduction of chemical compound space. Here, we demonstrate that the Martini model is not optimal for chemical transferability, and we propose new criteria for the rational design of coarse-grained models that allows for the optimization of their chemical transferability. We validate this hypothesis by parameterizing three Martini-like force fields, in which the number of bead types ranges from five to sixteen for the different force fields. We demonstrate that a level of performance and accuracy comparable to Martini can be obtained by using a force field with fewer bead types, thus making this force field more efficient at reducing the chemical compound space. Furthermore, constructing this force field with chemical transferability as a foundation allows us to know a priori the most likely chemistries that correspond to a specific bead type.

CPP 25.35 Tue 14:00 Poster B1

Hoobas: A python-based flexible molecular builder — •Martin Girard[1], Annaliese Ehlen[2], Anisha Shakya[2,3], Tristan Bereau[1], and Monica Olvera de la Cruz[2] — [1]Max Planck Institute for Polymer Physics, Mainz, Germany — [2]Department of Material Science and Engineering, Northwestern University, Evanston, IL, USA — [3]Center for Soft and Living Matter, Institude for Basic Science, Ulsan, South Korea

Molecular dynamics has emerged as a powerful and efficient tool to study soft matter. As the computing power available increases, so does the complexity of studied systems. In order to perform a simulation, initial positions and topologies must be built. A few tools already exist, but are generally very specific in terms of systems they can build. Here, we introduce Hoobas, a molecular building tool able to handle very general systems and nearly arbitrary polydispersity using a prototype-builder design pattern. As examples, we show building of DNA-coated colloidal crystals, lipid membranes and random hyperbranched polymer melts. The objects provided are easily extensible to other topologies.

CPP 25.36 Tue 14:00 Poster B1

Boehmite Microcrystal Growth and its Interaction with Polymers at the Interface. — •Mateusz Dudziak, Dorothee Silbernagl, and Heinz Sturm — Bundesanstalt für Materialforschung und prüfung (BAM), Berlin, Germany

Nanocomposites are extremely versatile due to their physicochemical properties, which differ significantly from bulk homopolymers. One of the inorganic nanomaterials, which is increasingly used as a filler in polymer matrices is boehmite, due to its flame-retardant properties. Here, it is utilized as a nanofiller in polycarbonate and polyamide, expecting to improve their mechanical properties. For industrial use boehmite is obtained by the solvothermal method, resulting in a layered nanomaterial, whereas naturally it occurs as single crystals with the size of <50*m. In this work we are obtaining and isolating boehmite monocrystals by a bottom-up method, in which a reaction between aluminum salts and hydroxides takes place in a polymer gel. Obtaining boehmite as microcrystals is necessary for its analysis and characterization, as well as to investigate its interaction with polymer matrices at the polymer/particle interface. Here, the obtained particles are characterized by small- and wide-angle X-ray scattering and further in polymer matrices with differential scanning calorimetry and intermodulation atomic force microscopy (ImAFM), probing local stiffness.

CPP 25.37 Tue 14:00 Poster B1

A different kind of True Random Number Generator - Stoachastic Assembly of Ag/Au Single Particle Lines — •Daniel Schletz[1], Martin Mayer[1,2], Anja Maria Steiner[1,2], and Andreas Fery[1,2,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [2]Cluster of Excellence Center for Advancing Electronics Dresden, Germany — [3]Department of Physical Chemistry of Polymeric Materials TU Dresden, Germany

Standard hardware random number generators often use quantum mechanical phenomena or thermal noise to produce bit streams of random, but often biased, origin. In contrast, colloidal self-assembly of billions of particles on $1\,\mathrm{cm}^2$ can assure bias-free, heterogeneous particle sequences to be employed as bits in a hardware random number generator.

Utilizing template-assisted colloidal self-assembly of two different particle types (Au spheres and Ag spheres), heterogeneous single particle lines are assembled and subsequently analyzed *via* electron microscopy. Statistical evaluation shows that Ag and Au do not assemble in any way preferential to any particle type, generating random distributions only dependent on employed Ag/Au particle share.

CPP 25.38 Tue 14:00 Poster B1

Synthesis of protein-coated gold nanoparticles and investigations on their uptake by diatoms — •Marisa Hoffmann[1,2], Nathalie Pytlik[1], Roland P. M. Höller[2], Christian Kuttner[2], Andreas Fery[2,3], and Eike Brunner[1] — [1]Department of Bioanalytical Chemistry, TU Dresden, Germany — [2]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [3]Department of Physical Chemistry of Polymeric Materials, TU Dresden, Germany

Because of the inertness and the surface plasmon resonance (SPR) of gold nanoparticles (AuNPs) and the biocompatibility of natural proteins, the combination of both provides a promising system for *in vivo* surface enhanced Raman spectroscopy (SERS) applications. AuNPs were synthesized by the citrate reduction method and the kinetically controlled seeded growth of citrate-stabilized AuNPs (Bastús 2011). Ligand exchange of the citrate by bovine serum albumin (BSA) was then performed. Gold/gold 3D core/satellite nanoclusters were synthesized by protein assisted self-assembly in solution (Höller 2016). After incubating cells of the diatom species *stephanopyxis turris* with the mentioned protein-coated AuNPs and gold nanoclusters, respectively, *in vivo* 3D Raman imaging was carried out. As, for a detectable SERS enhancement, plasmonic nanostructures in the vicinity of the analyte are necessary, the localization of AuNPs can be determined by the position of the SERS signals. That way it was possible to successfully investigate the uptake of AuNPs and gold nanoclusters by the diatom cells. This opens up the way for a new method in prospective *in vivo* research of algal metabolism.

CPP 25.39 Tue 14:00 Poster B1

Dynamic Fluorescence Properties of Graphene Quantum Dots — •Christian Wimmenauer[1], Ralf Künemuth[2], Stefan Fasbender[1], Claus A M Seidel[2], and Thomas Heinzel[1] — [1]Institute of Experimantal Condensed Matter Physics, Heinrich-Heine-University Düsseldorf — [2]Institute of Physical Chemistry, Heinrich-Heine-University Düsseldorf

Graphene quantum dots (GQDs) are a promising candidate for various biomedical applications ranging from drug delivery to single particle tracking, due to their small size and low toxicity. To characterize GQDs concerning their viability as a fluorescence marker time correlated single photon counting and fluorescence correlation spectroscopy are employed. The fluorescence lifetime, the time scales of different dark states and the diffusive properties are determined. Dark states are discussed for coupled and uncoupled GQDs at different pH values. The measured properties allow for an assessment of the usability in biomedical applications, such as single particle tracking or super resolution microscopy.

CPP 25.40 Tue 14:00 Poster B1

Energy Spectra of Triangular Multilayer Graphene Quantum Dots — •Julienne Scheller, Christian Wimmenauer, and Thomas Heinzel — Institute of Experimantal Condensed Matter Physics, Heinrich-Heine-University Düsseldorf

Triangular Multilayer Graphene Quantum Dots (GQDs) are modelled using a tight binding approach. The energy gaps are calculated as a function of disk radius, number of disk layers and edge type. Armchair edge type and zigzag edge type GQDs are investigated for up to 7 layers and in the limit of infinitely many layers. To further discuss the differences between both edge types the density of states and the ground state wavefunctions are calculated.

CPP 25.41 Tue 14:00 Poster B1

Momentum Space Calculations of Nano Scaled Semiconductor Materials — •Marcel Dohrmann, Christian Strelow, and Alf Mews — Institute of Physical Chemistry, University Hamburg, Grindelalle 117, 20146 Hamburg, Germany

Excitons energy calculations are done by solving Schrödinger's equations of kinetic terms, including the effective mass of electrons and holes, and potential terms. In position space, three-dimensional self-consistent calculations with hole and electron functions are used to understand different nano sized semiconductors like CdSe/CdS dot-rods.[1] Using fourier transformations the kinetic and potential Hamiltonians in position space can be adapted to momentum space. A potential landscape in momentum space is an approach to calculate energy levels of electrons and holes in different composites. We see forward to study interaction between heavy and light holes in semiconductor nanomaterials.

[1] S.-H. Lohmann, C. Strelow, A. Mews, T. Kipp, ACS Nano 2017, DOI 10.1021/acsnano.7b05303.

CPP 25.42 Tue 14:00 Poster B1

A Combined SAXS-SANS instrument at ILL — •Ezzeldin Metwalli, Klaus Götz, Christian Bär, and Tobias Unruh — Institute for Crystallography and Structural Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

In the last few decades, small angle X-ray and neutron scattering (SAXS/SANS) methods have been used extensively for investigating nano-scale structured materials. Combining both SAXS and SANS techniques in a single experiment will open a new route for a novel nano-analytical method. Simultaneous SAXS and SANS measurements will provide structural information from the same sample volume allowing unique different contrast conditions. Moreover, exploiting X-ray and neutron radiation for time-resolved studies will simultaneously provide nano-scale structural information at two different contrast situations, ensuring the exactness of the probed samples compared with independent experimental approach. Here, we introduce an advanced portable SAXS system that is dimensionally suitable to be installed on D22 instrument at ILL. The new portable SAXS system is based on Copper/Molybdenum switchable microfocus rotating anode X-ray generator and a Dectris detector with a changeable sample-to-detector distance of up to 1.5 m in a vacuum tube. The unprecedented combined experimental approach using simultaneous SAXS/SANS methods will open the way for investigating a truly wide range of innovative materials such as smart self-assembling nanomaterials, multifunctional materials, and organic/inorganic hybrid nanomaterials.

CPP 25.43 Tue 14:00 Poster B1

Self-assembly in magnetic filament systems: impact of internal factors — Elena Pyanzina, Tatyana Belyaeva, Marina Kashpurova, and •Ekaterina Novak — Ural Federal University

The fundamental understanding of the self-assembly properties of colloidal systems is one of the key topics in current research on novel microstructured soft materials and technologies. In this work we investigate self-assembly of magnetic filaments of different topology with different additional interaction and particles polydispersity. We performed molecular dynamics simulations using a Langevin thermostat. Cluster analysis based on graph theory is used to analyze the obtained data. At the moment we are analyzing the results, but we can already say that the introduction of additional attraction and particles polydispersity significantly expands the structural diversity of the self-assembly of magnetic filaments, and the effect of magnetic dipole-dipole interaction remains substantial. All these results will pave the way for the development of analytical models and identify the most interesting building block candidates for the design of new magnetoresponsive materials.

CPP 25.44 Tue 14:00 Poster B1

Equilibrium behavior of surface-grafted supracolloidal ferromagnetic filaments — •Pedro A. Sánchez[1,2], Joan J. Cerdà[3], Tomás Sintes[4], and Sofia S. Kantorovich[1,2] — [1]Computational Physics, University of Vienna, Vienna, Austria — [2]Ural Federal University, Ekaterinburg, Russia — [3]IAC3, Universitat de les Illes Balears, Palma de Mallorca, Spain — [4]Instituto de Física Interdisciplinar y Sistemas Complejos, UIB-CSIC, Palma de Mallorca, Spain

Supracolloidal magnetic filaments, that are semiflexible chains of magnetic micro- or nanoparticles permanently crosslinked by polymers, are used for the creation of magnetically driven microfluidic propellers and pumpers, micromechanical sensors and contrast imaging agents. These systems have been also proposed as building blocks of thin films that can change their structure and rheological properties as a response to external magnetic fields. Most of such applications involve the interaction of free or end grafted filaments with inert or attracting surfaces.

Here we study, by means of computer simulations, the equilibrium structures of individual magnetic filaments made of ferromagnetic particles when placed near to interacting flat surfaces. We focus on the structural changes that take place on cooling depending on the strength of the interaction with the surface and the applied field, comparing the cases of free and grafted filaments.

CPP 25.45 Tue 14:00 Poster B1

Light-induced deformation of azo-polymer droplets - challenges in modelling the influence of light — •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, Germany

In recent years azobenzene-containing materials have been gaining a lof of scientific interest due to the possibility to change their properties by using light as an external stimulus [1]. These effects are based on the trans-cis photoisomerization of azobenzene and its interplay with the surrounding system. To gain a deeper understanding of the deformation of azo-materials we study an azo-polymer droplet on a silica surface exposed to UV-vis light. Here, the azo side groups of the polymer chains reorient perpendicular to the E-field of light due to cyclic photoisomerization [2]. Using MD simulations we study the influence of linearly polarized light on the droplet applying two different approaches. In the first case we simulate the repeated angle-dependent trans-cis photoizomerization of azobenzenes explicitly by temporally changing the torsion angle around the azo bond [3]. In the second case we utilize an effective orientation potential [2], which reorients the azobenzenes without modelling the photoisomerization events.

We gratefully acknowledge support from German Research Foundation (DFG), projects GU 1510/3-1 and SA 1657/13-1.

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[2] Toshchevikov, V. et al. J. Phys. Chem. B, 113(15), 5032 (2009)
[3] Heinz, H. et al. Chem. Mater. 20, 6444 (2008)

CPP 25.46 Tue 14:00 Poster B1

Structure and Switching of Azobenzene Layers Physisorbed on Mica and Glass — •Amrita Pal[1], Olga Guskova[1], Alexey Kopyshev[2], and Svetlana Santer[2] — [1]Institute Theory of Polymers, IPF Dresden, Germany — [2]Institute of Physics and Astronomy, University of Potsdam

We study the photoswitchable amphiphilic molecules [1] with charged trimethyl ammonium head group and the hydrophobic tail consisting of alkyl and azobenzene (azo) segments. Being physisorbed on mica or glass surfaces, these molecules build the self-assembled monolayers. The reversible photoswitching of thickness of the layers is investigated in both AFM experiments and DFT/MD simulations. The in-situ AFM experiments show that the photoisomerization of the azo molecules under irradiation with light of different wavelength results in significant change of morphology, i.e. thickness and topography of azo multilayers. In DFT, the triple zeta basis set and generalized gradient approach, hybrid and range separated hybrid functionals are used to obtain the isomeric properties at the molecular level. Also, a periodic DFT calculation is performed for a single molecule adsorbed onto a small mica cluster to compare the results of quantum and classical simulations. The DFT calculations of the azo isomers in vacuum and in adsorbed state reveal the influence of the surface on their electronic properties. The MD simulation of denser layers consisting of many azo molecules uncovers their detailed structures and allows a direct comparison with AFM data. We acknowledge support from DFG, GU 1510/5-1. [1] Montagna, M. et al. Langmuir 34(1), 311 (2018)

CPP 25.47 Tue 14:00 Poster B1

Water dynamics in a concentrated poly(N-isopropylacrylamide) solution at high pressure — •Bart-Jan Niebuur[1], Wiebke Lohstroh[2], Marie-Sousai Appavou[3], Alfons Schulte[4], and Christine M. Papadakis[1] — [1]TU München, Physik Department, Garching, Germany Physik weicher Materie, — [2]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Garching, Germany — [3]FZ Jülich, JCNS at MLZ, Garching, Germany — [4]University of Central Florida, Department of Physics and College of Optics and Photonics, Orlando, U.S.A.

Hydration water is of fundamental importance for the phase transitions of macromolecules in aqueous solution. A complete picture of the dynamics of hydration water is therefore key for identifying the processes involved. Using quasi-elastic neutron scattering, we study the hydration behavior of a concentrated solution of the thermoresponsive polymer poly(N-isopropylacrylamide) during heating through its cloud point (CP). Varying pressure alters its hydration state [1]. At low pressure, the fraction of hydration water decreases sharply at the CP. The diffusion of the remaining fraction gets increasingly hindered, which points to a rearrangement of the hydration water. In the one-phase state at high pressure, the hydration water diffuses more rapidly than at low pressure, which indicates enhanced hydrophobic hydration. At the CP, the fraction of hydration water decreases by a similar amount as at low pressure, but the transition spans over ∼10 K. At high pressure, the hydrophobic groups stay hydrated in the two-phase state. [1] B.-J. Niebuur, C. M. Papadakis et al., *ACS Macro Lett.* 2017, **6**, 1180

CPP 25.48 Tue 14:00 Poster B1

Mesoglobules in PNIPAM solutions: Influence of pressure — Bart-Jan Niebuur[1], •Geethu P. Meledam[1], Vitaliy Pipich[2], Marie-Sousai Appavou[2], Alfons Schulte[3], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]FZ Jülich, JCNS at MLZ, Garching, Germany — [3]University of Central Florida, Orlando, U.S.A.

Poly(N-isopropylacrylamide) (PNIPAM) in aqueous solution forms mesoglobules upon heating through the cloud point, which are small and contain only little water. In contrast, at high pressure, much larger clusters are formed, which contain more water than at atmospheric pressure [1]. We use very small angle neutron scattering at temperatures above the cloud point to elucidate the transition between low and high pressures. We find a sharp transition between small mesoglobules and large clusters with the transition pressure depending on temperature. We attribute the pressure-dependent behavior on mesoscopic length scales to the pressure-dependent hydration of PNIPAM.

1. B.-J. Niebuur et al., ACS Macro Lett. 6, 1180 (2017)

CPP 25.49 Tue 14:00 Poster B1

Preferential binding of salts to pNiPAM and its monomer — •Jakub Polák, Adam Kovalčík, Pavel Vrbka, Daniel Ondo, Vladimír Palivec, and Jan Heyda — Department of Physical

Chemistry, University of Chemistry and Technology, Prague, Czech Republic

Over past decade investigation of salt specific effects on biomolecules attracted a lot of experimental, computational and theoretical attention. However, the direct quantitative thermodynamic characterization is still poor. In this contribution we measure a preferential binding coefficient of salts to a well established model biomolecule, poly-N-isopropyl-acrylamide (pNiPAM). The pNiPAM-salt interaction is determined in equilibrium dialysis experiments. The results are supplemented by vapor pressure osmometry experiments of NiPAM, in which salt-monomer interactions at dilute conditions were determined. Finally, in combination with density measurements and upon application of theory of solution the thermodynamically relevant basic ingredients, Kirkwood-Buff integrals, were determined.

CPP 25.50 Tue 14:00 Poster B1

Simulating the hydrodynamics of droplets on photo-switchable substrates — •Josua Grawitter and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

Photo-switchable substrates provide a unique mechanism to manipulate liquid droplets precisely by creating and adapting a heterogeneous wettability landscape. Because droplets respond to changes in the wettability, this is a means to keep them in non-equilibrium and thereby induce new states of dynamic wetting.

We present a boundary element method to determine the Stokes flow inside the droplet with a curved free surface and a flat interface at the substrate, where we apply the Navier boundary condition to permit motion of the contact line. In general, boundary element methods solve integral equations by inverting the discretized integrals of the unknown field variable such as fluid velocity.

In our approach we parametrize the free surface of the droplet by a linear combination of smooth basis functions and, using an automatic differentiation algorithm, we calculate its local metric and curvature. This provides high resolution data for an iterative domain-splitting integration scheme capable of treating singular integrands, which are typical for the boundary element method. Following rigorous validation, we will investigate how droplets respond to specific spatio-temporal wettability patterns that either move or deform the droplet. For example, we will generate directed motion by traveling patterns and vary their properties to maximize droplet speed.

CPP 25.51 Tue 14:00 Poster B1

Stable 2D conductive and transparent metal/metal(hydr)oxide multilayers prepared by manipulated wetting — •Sebastian Runde, Heiko Ahrens, Harm Wulff, and Christiane A. Helm — Institute of Physics, Universität Greifswald, Felix-Hausdorff-Str. 6, 17489 Greifswald

We present a new deposition method allowing ultrathin, conductive and transparent metal-containing layers to be prepared at ambient conditions with cm^2 areas on glass substrates. Multilayers are formed by repetition of the deposition procedure, induced break-up after forced wetting. Different liquid metals and their alloys, Bismuth, Gallium, Indium and Tin were used and compared. These metals all have a low melting temperature, a high wettability and form instantaneously a passivating oxide skin. X-ray measurements show that multilayer thickness increases linearly with the number of deposition cycles, yielding a reproducible single layer thickness between 3 and 6 nm. The largest layer number achieved was 13 (54 nm thick). The sheet resistance and the optical absorbance decrease monotonically with the number of deposited layers.

CPP 25.52 Tue 14:00 Poster B1

Buckling patterns and their elastic response on the surface of polyelectrolyte multilayer films with short PSS chains — •Amir Azinfar[1], Sven Neuber[1], Jiří Vaněček[2], Marie Vancová[2,3], Jan Sterba[2,3], Vítězslav Straňák[3], and Christiane A. Helm[1] — [1]Institute of Physics, University of Greifswald, 17489 Greifswald, Germany — [2]Biology Centre, Czech Academy of Sciences, 37005 Ceske Budejovice, Czech Republic — [3]Faculty of Science, University of South Bohemia, B 37005 Ceske Budejovice, Czech Republic

We investigate the surface morphology of polyelectrolyte multilayers (PEMs) after drying. A buckling pattern is observed. PEMs are made from poly(diallyldimethylammonium (PDADMA) and poly(styrene sulfonate) (PSS) in 0.1 M NaCl with non-linear and linear growth regimes. When more PSS/PDADMA layer pairs are deposited, for PSS-terminated films the wavelength of the buckling pattern increased from 185 nm to 225 nm. For PDADMA-terminated films the wavelength was always greater. The buckling pattern is correlated with the elastic modulus of the film, which decreased with increasing film thickness. Annealing in high salt concentrations (0.5 -1.0 mol/l NaCl) decreased the surface roughness and increased the wavelength of the buckling pattern. However, for films containing mobile PSS, annealing caused a damped oscillation of the buckling pattern.

CPP 25.53 Tue 14:00 Poster B1

Wetting and imbibition experiments with aqueous electrolyte solutions and polymers on nanostructured and porous materials — •Guido Dittrich and Patrick Huber — Institute of Materials Physics and Technology, Hamburg University of Technology (TUHH), Eißendorfer Str. 42, D-21073 Hamburg-Harburg, Germany

Nanostructured as well as porous materials offer high specific surface areas per projected area and volume respectively. That makes them interesting for fundamental research since the discovery of super hydrophobicity and super permeation. We are investigating the imbibition kinetics of polystyrene into porous scaffold materials comparing different pore systems. The imbibition kinetics are measured with a gravimetric and an interferometric setup. Analysis of aqueous electrolyte solution droplets may lead to fast tests to get insights regarding surface roughness, successful chemical impregnation and interface fractions. Commercially available p-doped silicon wafers can be nanostructured by electrochemical etching. We seek to overcome their tendency to increase their native oxide layer during electrowetting experiments by chemical modification of the surfaces end groups. Dynamic wetting on carbon nanotube (CNT) arrays glued together by epoxy is driven by capillarity. After the synthesis the CNTs are opened by different techniques. Drop shape analysis is used to supplement scanning electron microscopy to verify open pores.

CPP 25.54 Tue 14:00 Poster B1

Hard sphere electrolyte solution at charged wall — •Maximilian Mussotter[1], Markus Bier[2], and S. Dietrich[1] — [1]Max-Planck Institut für Intelligente Systeme und Universität Stuttgart, 70569 Stuttgart, Germany — [2]University of Applied Sciences Würzburg-Schweinfurt, 97421 Schweinfurt, Germany

Although widely used, upon advancing from electrically neutral fluids and uncharged subtrates, the assumption of homogeneous wall-fluid interactions is questionable beyond molecular length scales when studying fluids comprising electrically charged constituents and charged walls. Therefore, the intention of this work was to gain further insight in the effects occurring at non-uniformly charged substrates. The system is studied by means of classical density functional theory, within the framework of fundamental measure theory using the WBI-functional. The goal of this work was to introduce a basic machinery to study the effects of nonhomogeneously charged surfaces.

CPP 25.55 Tue 14:00 Poster B1

Microscopic investigation of polymer flow in porous media — •Pegah Shakeri[1,2], Michael Jung[1,2], Martin Brinkmann[1], Stephan Herminghaus[2], and Ralf Seemann[1,2] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Max Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

The displacement of a fluid from a permeable medium by injecting a second immiscible fluid is central in many industrial processes like oil recovery. The general assumption is that the polymer modifies the viscosity of the injected fluid; thus improves the volumetric sweep efficiency (the amount of displaced oil) by enhancing mobility ratio and controlling viscous fingering in macro scale. However, recent observations suggest that additionally microscopic effects are important; thus microscopic investigation of a polymer flow in a quasi-2D microfluidic device was conducted to gain clear insight into the pore scale mechanism of oil displacement by a polymer solution in permeable media. Deviation from laminar flow, fluctuating oil-polymer solution interfaces, lower residual saturation in comparison to a flood of water or aqueous glycerol solution (having the same zero shear viscosity as the polymer solutions) were observed. The observed instabilities in the bulk flow,which seem to originate from viscoelasticity of the polymer solution, destabilize the oil-polymer interface and are consequently capable of improving the microscopic displacement.

CPP 25.56 Tue 14:00 Poster B1

Monitoring Pressure Fluctuations in Artificial Porous Media. — •Michael Jung[1,2], Martin Brinkmann[1], Stephan

Herminghaus[2], and Ralf Seemann[1,2] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Max Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

We aim to understand the microscopic mechanisms of individual capillary instabilities which govern slow displacement processes in permeable porous media. Therefore we investigate the influence of the pore space geometry and wettability on the landscape of pressure variations during slow displacement of fluid from an arrangement of glass beads by a second, immiscible fluid. For an experimental verification of the capillary pressure variations, we measure the pressure of a bursting meniscus in a single throat formed by three beads. Different wettability of the glass beads is realized by wet-silanization techniques as OTS (octadecyltrichlorosilane) or APTES (3-aminopropyltriethoxysilane)-coating which result in a water-air contact angle on glass beads of 110° and 60°, respectively. Heterogeneous wettability is achieved by throats assembled from beads with different coatings. The experiments shall be compared with numerical calculations of the capillary pressure in such a heterogeneous throat for various combination of contact angles. Understanding the characteristic pressure variations of single throats, we will extend our setup to small bead-packs consisting of a few layers of glass beads with heterogeneous wettability.

CPP 25.57 Tue 14:00 Poster B1

A fast quartz crystal microbalance (QCM) with millisecond time resolution operating on multiple overtones at the same time — •Arne Langhoff, Frederick Meyer, Astrid Peschel, Judith Petri, and Diethelm Johannsmann — Institut für Physikalische Chemie, TU Clausthal, Germany

Second-generation QCMs (which include the QCM-D) rely on readings of the resonance frequency as well as bandwidth on multiple overtones. The added information gives access to the sample's softness and other properties. Currently, most QCMs need about a second per frequency reading and they access different overtones sequentially. Using a multi-frequency lockin amplifier (MLA, supplied by Intermodulation Products AB, Stockholm), this limitation can be overcome. The MLA excites the resonator at 40 frequencies simultaneously. The channels are distributed over four "combs" (10 frequencies each), where each comb covers one overtone. The time resolution can be close to the inverse resonance bandwidth, which - for high-fundamental-frequency (HFF) resonators - is well below one millisecond. The technique is particularly powerful when applied to repetitive processes because accumulation can then lower the noise in frequency shift of 5-MHz resonators well into the mHz range. Applications chosen for demonstration are the impact of droplets onto the QCM surface (the kinetics of which is in ms range) and electrochemical measurements (in which case accumulation and averaging can be exploited). In the latter case, the fast dynamics after voltage reversal is monitored. The response is governed by changes of viscosity in the double layer.

CPP 25.58 Tue 14:00 Poster B1

Water freezing and frosting on lubricant impregnated surfaces — •Lukas Hauer[1,2] and William Wong[1] — [1]Max Planck Institute for Polymer Research — [2]Institute of Fluid Mechanics and Aerodynamics, Technische Universität Darmstadt

In the scope of the present work, frost formation and drop freezing in/on lubricant-infused surfaces (”under-oil” dynamics) are experimentally investigated. Glass substrates structured with SU-8 micropillar arrays are chosen as model surfaces. To examine frost formation, a sample is placed on a Linkam peltier stage which is enclosed in a chamber with humidity control to induce condensation-frosting. To examine freezing, the sample (and deposited drop) is placed in an alternate chamber with temperature control, which is cooled using liquid nitrogen. Frost formation and drop freezing will be observed using an inverted laser scanning confocal microscope. This spatially and temporally resolved technique allows accurate observation of these dynamic processes close to the substrate surface. By adding a dye to the lubricant, the water-lubricant interfaces can be discriminated, allowing us to monitor lubricant mobility during freezing/frosting. During frost formation, a migration of the lubricant to the top of the ice has been observed. Due to the dendritic morphology of frost, capillary effects are believed to be the driving forces of this phenomenon. Such effects could lead to lubricant drainage and failure of surface functionality. A fundamental understanding of the lubricant migration will help to design more ice-durable slippery surfaces.

CPP 26: Active Matter B (joint session DY/CPP)

Time: Tuesday 14:00–15:45 Location: H3

CPP 26.1 Tue 14:00 H3

Collective behavior of active colloids in confined viscoelastic fluids — •N Narinder[1], Mahsa Sahebdivani[1], Juan Ruben Gomez-Solano[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Instituto de Física, Universidad Nacional Autónoma de México, México.

The natural habitat of microorganisms is complex not only in geometrical aspects but also in the sense that it is viscoelastic [1]. The fundamental question to address is what prime role such sophisticated surroundings play. To uncover this, we experimentally study the motion of light activated Janus particles in a viscoelastic fluid inside hard wall circular confinements. Unlike a Newtonian liquid [2], we observe that particles in viscoelastic fluids [3] experience an elastic repulsion from the walls which strongly depends on their activity and the elasticity of the surrounding fluid. Furthermore, strongly confined many-particle system inside circular pores exhibits a transition from liquid-like to a well-organized crystal-like behavior upon increasing the activity of particles. A further increase in activity liquifies the system and thus a reentrant liquid-like behavior is observed.

[1] J. Elgeti, R. G. Winkler, and G. Gompper, Rep. Prog. Phys. 78, 056601 (2015).

[2] G. Volpe, I. Buttinoni, D. Vogt, H. Kümmerer and C. Bechinger, Soft Matter 7, 8810 (2011).

[3] N. Narinder, C. Bechinger, and J. R. Gomez-Solano, Phys. Rev. Lett. 121, 078003 (2018).

CPP 26.2 Tue 14:15 H3

Two-step melting in two-dimensional active matter — Juliane Klamser[1], •Sebastian Kapfer[2], and Werner Krauth[1] — [1]Laboratoire de Physique Statistique, Département de physique de l'ENS, Ecole Normale Supérieure, Paris, France — [2]Theoretische Physik 1, FAU Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany

Phase transitions in active matter offer a window to study the elusive critical phenomena outside equilibrium and have taken the center stage of studies in modern statistical physics. We present a kinetic Monte Carlo model of interacting active particles which can be connected to the equilibrium phase diagram. Using extensive numerical simulations, we show that this active model exhibits a rich phase behavior, including liquid-gas coexistence (motility induced phase separation) and the first ever evidence of two-stage melting via solid-hexatic-liquid outside equilibrium.

CPP 26.3 Tue 14:30 H3

Self-organized large-scale order in active fluids — Martin James[1,2], Dominik Suchla[1,2], and •Michael Wilczek[1] — [1]Max-Planck-Institut für Dynamik and Selbstorganisation, Göttingen — [2]Georg-August-Universität Göttingen

Active fluids, such as dense suspensions of bacteria or microtubules and molecular motors, display a fascinating range of dynamical states. Active stresses exerted by the individual agents, along with their hydrodynamic interactions, generically lead to the emergence of mesoscale vortex patterns reminiscent of two-dimensional turbulence. In this presentation, we discuss how ordered flows emerge in a minimal continuum model of active fluids. In particular, we focus on a novel type of turbulence-driven pattern formation: a self-organized, dynamic vortex crystal. Crucially, this state emerges from an extended disordered transient characterized by an upscale energy transfer. Exploring the transition from active turbulence to the vortex crystal state with a focus on the role of fluctuations and system size, we find surprising analogies to classical phase transitions. For example, we observe locally ordered crystal domains, which share similarities with magnetic domains in ferromagnetic materials, separated by turbulent boundaries. Our results therefore explore one route to self-organization in active flows.

CPP 26.4 Tue 14:45 H3

Dynamics of confined phoretic colloids — •Prathyusha Kokkoorakunnel Ramankutty, Suropriya Saha, and Ramin Golestanian — Max Planck Institue for Dynamics and Self Organization, Am Fassberg 17, Gottingen, Germany

Phoretic colloids are known to form clusters by mechanisms similar to those in black holes formed by long ranged gravitational forces. The long ranged interactions are driven by phoretic response of one colloid to the chemical field generated by others. We investigate the dynamics of uniformly coated colloidal assembly in a confined geometry using Brownian dynamics simulation. In steady state, the colloids self assemble to form a cluster and exhibits slow spontaneous fluctuations. The interesting cluster dynamics is studied as a function of number of particles and strength of phoretic interaction. The mean square displacement shows distinct plateaus indicating cage breaking dynamics.

CPP 26.5 Tue 15:00 H3

Continuum model for active polar fluids with density variations — •Vasco M. Worlitzer[1], Avraham Be'er[2], Gil Ariel[3], Markus Bär[1], Holger Stark[4], and Sebastian Heidenreich[1] — [1]Department of Mathematical Modelling and Data Analysis, Physikalisch-Technische Bundesanstalt, 10597 Berlin, Germany — [2]Zuckerberg Institute for Water Research, The Jacob Blaustein Intitutes for Desert Research, Ben-Gurion University, Sede Boqer Campus, Midreshet Ben-Gurion, Israel — [3]Department of Mathematics, Bar-Ilan University, Ramat Gan, Israel — [4]Institute of Theoretical Physics, Technical University of Berlin, 10623 Berlin, Germany

Bacterial suspensions are intriguing examples for active polar fluids which exhibit large scale collective behavior from mesoscale turbulence to vortex lattices. For dense bacterial suspensions an effective fourth-order polar field theory was introduced modelling the collective dynamics in agreement with experimental findings [1,2]. However, in recent experiments of Bacillus subtilis suspensions anomalous velocity statistics and density variations are found which are not captured by the theory. In our contribution, we present a phenomenological theory for an active polar fluid with density and swimmer-velocity variations. We show that these variations result in an anomalous velocity statistics as observed in recent experiments [3].

[1] J Dunkel, S Heidenreich, K Drescher, HH Wensink, M Bär and RE Goldstein, Phys. Rev. Lett. 110 (2013) 228102. [2] S Heidenreich, J Dunkel, SHL Klapp and M Bär, Phys. Rev. E 94 (2016) 020601(R). [3] SD Ryan, G Ariel, A Be'er, Biophys J. (2016) 247.

CPP 26.6 Tue 15:15 H3

Systematic extension of the Cahn-Hilliard model for motility-induced phase separation — Lisa Rapp, •Fabian Bergmann, and Walter Zimmermann — Universität Bayreuth, Germany

We consider a continuum model for motility-induced phase separation (MIPS) of active Brownian particles [J. Chem. Phys. **142**, 224149 (2015)]. Using a recently introduced perturbative analysis [Phys. Rev. E **98**, 020604(R) (2018)], we show that this continuum model reduces to the classic Cahn-Hilliard (CH) model near the onset of MIPS. This makes MIPS another example of the so-called active phase separation. We further introduce a generalization of the perturbative analysis to the next higher order. This results in a generic higher order extension of the CH model for active phase separation. Our analysis establishes the mathematical link between the basic mean-field MIPS model on the one hand, and the leading order and extended CH models on the other hand. Comparing numerical simulations of the three models, we find that the leading order CH model agrees nearly perfectly with the full continuum model near the onset of MIPS. We also give estimates of the control parameter beyond which the higher order corrections become relevant and compare the extended CH model to recent phenomenological models.

CPP 26.7 Tue 15:30 H3

Spatially periodic patterns succeed active phase separation — •Lisa Rapp, Fabian Bergmann, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth

We investigate a model equation for a conserved order-parameter field that covers as special cases the conserved Swift-Hohenberg model and the extended Cahn-Hilliard model for active phase separation. This model shows a primary bifurcation from a homogeneous state to large-scale phase separation - as typical for active phase separation [1,2]. We show here that with increasing distance from the primary bifurcation, however, a novel secondary bifurcation to spatially periodic patterns occurs. We explore these secondary periodic patterns in more detail including hysteresis and bistability/coexistence of patterns.

[1] F. Bergmann et al.: Phys. Rev. E 98, 020603(R) (2018)
[2] L. Rapp et al.: arXiv:1901.03203 (2019)

CPP 27: Plasmonics II (joint session O/CPP)

Time: Tuesday 14:00–16:30 Location: H8

CPP 27.1 Tue 14:00 H8

Sum-Frequency Generation Enhanced by Localized Surface Phonon Polaritons — •Riko Kiessling[1], Yujin Tong[1], Alexander J. Giles[2], Joshua D. Caldwell[2,3], Martin Wolf[1], and Alexander Paarmann[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]U.S. Naval Research Laboratory, Washington, D.C., USA — [3]Vanderbilt University, Nashville, USA

Nanophotonic devices open the way to tailor light-matter interaction on the nano-scale by specifically designed structures of solid-state material. This is advantageous for, e.g., the sub-diffractional localization of light, which fosters amplification of nonlinear optical frequency conversion processes by enhancement of local electric fields.

Here, we employ localized surface phonon polariton modes in nanostructured polar dielectric media [1] to resonantly increase the nonlinear response. In contrast to surface plasmons, the optical phonon-based approach exhibits significantly lower optical losses. By means of IR-VIS sum-frequency generation spectroscopy [2], a strong modulation of the local electromagnetic fields, and thus, amplified up-conversion radiation, is observed. Intensity and spectral position of the nonlinear emission can be manipulated by the nanostructure design. In this way, sub-wavelength sized architectures prove to be an efficient method for the control of localized fields associated with three-dimensionally confined optical modes in the mid-infrared spectral region.

[1] Razdolski et al., Nano Lett. 16, 6954 (2016)
[2] Kiessling et al., Phys. Rev. Accel. Beams 21, 080702 (2018)

CPP 27.2 Tue 14:15 H8

Nonlinear Response of Grating-Coupled Surface Phonon Polaritons — Marcel Kohlmann, Nikolai Christian Passler, Martin Wolf, and •Alexander Paarmann — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Surface Phonon Polaritons (SPhPs) have recently attracted much attention in infrared nanophotonics, due to their low losses compared to plasmon polaritons. Specifically for nonlinear optics, SPhPs result in tremendous enhancement of local optical fields [1,2]. Here, we study the nonlinear response of grating-coupled SPhPs [3] in by means of second-harmonic generation (SHG), in sub-wavelength SiC grating geometries. Non-specular emission of SHG is observed for resonant SPhP excitation, demonstrating the peculiarities of nonlinear scattering for grating-coupled nonlinear nanophotonics [4].

[1] Razdolski et al., Nano Letters 16, 6954 (2016).
[2] Passler et al., ACS Photonics 4, 1048 (2017).
[3] Greffet et al., Nature 416, 61 (2002).
[4] Quail and Simon, J. Opt. Soc. Am. B 5, 325 (1988).

CPP 27.3 Tue 14:30 H8

Wavelength-dependent Third Harmonic Generation in Metallic Thin Films — •Vincent Drechsler, Joachim Krauth, Mario Hentschel, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Harmonic generation in plasmonic systems has gained significant interest in the last years. While the plasmonic near-field enhancement has been studied in great detail, little attention was paid to the origin of the nonlinear signals which in fact lie in the microscopic nonlinearity of the involved plasmonic metals. In order to predict wavelength-dependent nonlinear processes it is therefore crucial to understand these microscopic nonlinearities. Utilizing an optical parametric oscillator as a tunable broadband light source, we study wavelength-dependent third harmonic generation from metallic thin films made of Gold, Copper, and Magnesium. We find that the linear properties of the metallic films, that is their absorption, strongly influence the third harmonic generation efficiency. Optical transitions between the different bands lead to a resonant enhancement of the third order susceptibilities. Utilizing hydrogen to switch metallic magnesium to dielectric magnesium hydride we can tune the nonlinearity of thin films and observe the metallic-dielectric phase transition in the linear and nonlinear regime. We find complex relations between the linear transmittance and the radiated third harmonic, which provide new insights into the phase transition.

CPP 27.4 Tue 14:45 H8

Plasmonic analogue of Electromagnetically Induced Absorption Boosts Third Harmonic Generation — •Joachim Krauth, Mario Hentschel, Bernd Metzger, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

In three-dimensional nanostructures, the appropriate choice of geometry and materials allows for tailoring the linear optical properties in a vast range. In the so-called plasmonic dolmen structure the coupling between a bright and a dark state can be manipulated to realize the plasmonic analogue of electromagnetically induced absorption (EIA), resulting in an enhanced absorbance of the coupled system. In analogy to solid state nonlinear optics, in which the linear absorption spectra largely determine the nonlinear interaction, plasmonic EIA is therefore expected to boost nonlinear conversion efficiencies. We are reporting third harmonic generation spectroscopy results on a plasmonic EIA system. The radiated third harmonic signals can be understood when taking the intricate phase relation and coupling strength dependence of EIA into account. An appropriately modified anharmonic oscillator model based on the linear absorption spectra can describe the nonlinear response of our three-dimensional plasmonic structure. The design freedom associated with three-dimensional nanostructuring can provide further insight into the nonlinear response of complex plasmonic systems.

CPP 27.5 Tue 15:00 H8

Symmetry-forbidden second-harmonic generation in a fully centro-symmetric plasmonic nanocircuit — •Julian Obermeier[1], Tzu-Yu Chen[2], Thorsten Schumacher[1], Fan-Cheng Lin[2], Jer-Shing Huang[3,4,5], Chen-Bin Huang[2,5], and Markus Lippitz[1] — [1]University of Bayreuth, Germany — [2]National Tsing Hua University, Taiwan — [3]Leibniz Institute of Photonic Technology, Germany — [4]National Chiao Tung University, Taiwan — [5]Research Center for Applied Sciences, Taiwan

Nonlinear optical frequency conversion on the nanoscale remains a challenge, but may pave the path towards multi-functional optical circuits. Surface plasmon fields are highly spatially confined near the metal/dielectric interface and exhibit giant field enhancement. These two attributes are invaluable for nonlinear optics with plasmons. However, second-harmonic generation in bulk is forbidden in centrosymmetric materials such as typical noble metals. Past efforts concentrated on the broken symmetry at the surface in combination with an asymmetric shape of the particle. We introduce a new way of breaking the symmetry by a propagating mode of a plasmonic waveguide, a two-wire transmission-line. We demonstrate that an optical mode of correct symmetry is sufficient to allow SHG even in centro-symmetric structures made of centro-symmetric material. This is a new degree of freedom for on-chip nonlinear signal processing in nanophotonics.

CPP 27.6 Tue 15:15 H8

Resonant Field Enhancement of Epsilon Near Zero Berreman Modes in an Ultrathin AlN Film — •Nikolai Christian Passler[1], Ilya Razdolski[1], Joshua D. Caldwell[2], Martin Wolf[1], and Alexander Paarmann[1] — [1]Fritz-Haber-Institute of the MPG, Berlin, Germany — [2]Vanderbilt University, Nashville, USA

In nanophotonics, the strongly enhanced local optical fields of polaritonic modes are the driving force of nonlinear optical phenomena. In sub-wavelength thin polar dielectric films, a polaritonic Berreman mode arises at the longitudinal optical phonon frequency where the dielectric permittivity crosses zero [1]. Complementary to this radiative epsilon near zero (ENZ) mode, also an evanescent ENZ polariton is supported at large in-plane momenta [2], exhibiting similar properties. At resonance, the Berreman mode features an immense field enhancement, enabling to boost the efficiency of nonlinear nanophotonic applications like all-optical ultrafast switching.

Employing a mid-infrared free-electron laser, we investigate the second harmonic generation (SHG) of an ultrathin AlN layer on top of bulk SiC. The employed SHG spectroscopy [3] serves as a direct experimental probe of the tremendous field enhancement of the high-quality, strongly confined ENZ Berreman mode. With these properties, the AlN thin-film Berreman mode offers an appealing platform for the development of novel infrared nanophotonic devices.

[1] Vassant et al., Optics Express 20, 23971 (2012)
[2] Passler et al., Nano Letters 18, 4285 (2018)
[3] Paarmann et al., Applied Physics Letters 107, 081101 (2015)

CPP 27.7 Tue 15:30 H8

Enhanced second harmonic emission from zinc oxide nanoparticles infiltrated into the pores of gold nanosponges — •Jue-Min Yi[1], Dong Wang[2], Felix Schwarz[3], Jinhui Zhong[1], Abbas Chimeh[1], Anke Korte[1], Peter Schaaf[2], Erich Runge[3], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität, 26129 Oldenburg — [2]TU Ilmenau,98693 Ilmenau. — [3]TU Ilmenau, 98693 Ilmenau

We introduce zinc-oxide (ZnO)-functionalized porous gold (Au) nanoparticles which exhibit strong second harmonic (SH) generation around 400 nm by coupling surface plasmons (SPs) to ZnO excitons. The hybrid nanosystem consists of a thin layer (~10 nm) of ZnO incorporated into individual porous Au nanoparticles percolated with a three-dimensional (3D) network of 10-nm sized ligaments acting as nanoantennas and nanocavities.We have utilized a broadband and few-cycle ultrafast laser to generate coherent nonlinear emission from individual bare nanosponges and from ZnO-functionalized sponges. The third harmonic (TH) emission spectrum of Au/ZnO hybrid particles reveals a distinct red shift with respect to pure Au sponges. In contrast, a substantial broadening of the SH spectra and a distinct blue-shift is seen in the ZnO-functionalized nanosponges. It is demonstrated that SH emission around 400 nm, close to the ZnO band gap, is 15 times stronger with respect to bare Au nanosponges. Such enhanced SHG emission is attributed to plasmon-enhanced two-photon excitation of ZnO excitons.

CPP 27.8 Tue 15:45 H8

Revealing Plasmon-Exciton Coupling for SHG Enhancement by Interferometric Frequency Resolved Autocorrelation — •Jinhui Zhong[1], Juemin Yi[1], Dong Wang[2], Anke Korte[1], Abbas Chimeh[1], Peter Schaaf[2], and Christoph Lienau[1] — [1]Institute of Physics, Carl von Ossietzky University Oldenburg, 26129 Oldenburg, Germany — [2]Institut für Mikro- und Nanotechnologien Macro-Nano and Institut für Werkstofftechnik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Plasmon-enhanced excitonic nonlinear emission from semiconductors is interesting because the coupling of plasmon and exciton may boost the nonlinear generation efficiency. Nevertheless, to date, a detailed characterization of the electron dynamics of metal(plasmon)-semiconductor(exciton) composites is lacking. Herein, we present interferometric frequency-resolved autocorrelation (IFRAC) measurements on individual porous gold nanoparticles (nanosponges) incorporated with ZnO that allows us to track spectrally and temporally the response of the generated second-harmonic fields. We propose a method to distinguish homogeneous and inhomogeneous spectral broadening of plasmon resonances by Fourier-transform of the IFRAC traces to get two-dimensional (2D) IFRAC spectra. More importantly, we observed enhanced excitonic SHG emission at 390 nm from ZnO by coupling to localized plasmons of gold nanosponges. Pronounced features of coherent plasmon coupling are observed, proving that localized plasmons enhance the nonlinear ZnO excitonic emission, as revealed from the fundamental (FM) sidebands of the 2D spectra.

CPP 27.9 Tue 16:00 H8

Low-temperature infrared dielectric function of hyperbolic α-quartz — •Christopher J. Winta, Martin Wolf, and Alexander Paarmann — Fritz-Haber-Institut der Max-Planck-Gesellschaft

Natural hyperbolic materials, where the principal components of the dielectric tensor have opposite signs, like hexagonal boron nitride [1], have recently attracted much attention due to their unique characteristics for polaritonic nanophotonics [2]. Here, we show that also the common uniaxial crystal α-quartz exhibits multiple hyperbolic bands in the far-infrared (far-IR), which support low-loss hyperbolic modes at low temperatures.

We determine the IR dielectric properties of α-quartz in the temperature range from 1.5 K to 200 K. Far-IR reflectivity spectra of a single crystal y-cut were acquired in 8 distinct configurations. Fitting a multi-oscillator model globally to these data allows for extraction of frequencies as well as damping rates of the in-plane and out-of-plane, the longitudinal and transverse IR-active optic phonon modes, and hence the temperature-dependent ordinary and extraordinary dielectric functions, $\varepsilon_\perp(\omega)$ and $\varepsilon_\parallel(\omega)$, respectively.

The results are consistent with previous high temperature studies [3] and indicate remarkably high quality factors, Q, for polaritons at low temperatures in α-quartz's hyperbolic spectral region.

[1] Caldwell et al., *Nature Communications* **2014**, *5*.
[2] Liu, Lee, Xiong, Sun, Zhang, *Science* **2007**, *315*, 1686–1686.
[3] Gervais and Piriou, *Phys. Rev. B* **1975**, *11*, 3944–3950.

CPP 27.10 Tue 16:15 H8

Tunable Low Loss 1D Surface Plasmons in InAs Nanowires — •Yixi Zhou[1], Jianing Chen[1], and Thomas Taubner[2] — [1]Institute of Physics, CAS — [2]Institute of Physics (IA), RWTH Aachen

Due to the ability to manipulate photons at the nanoscale, plasmonics has become one of the most important branches in nanophotonics [1]. The prerequisites for the technological application of plasmons include high confining ability (λ_0/λ_p), low damping, and easy tunability. However, plasmons in typical plasmonic materials, i.e. noble metals, cannot satisfy these three requirements simultaneously, therefore limiting their overall applicability [2].

Here, indium arsenide (InAs) nanowires are identified as a material that satisfies all three prerequisites, providing a platform for modern nanophotonics. The dispersion relation of InAs plasmons is determined using the nanoinfrared imaging technique, and show that their associated wavelengths and damping ratios can be tuned by altering the nanowire diameter and dielectric environment. The launched plasmons simultaneously exhibit high confinement factor ($\lambda_0/\lambda_p = 34$) and low damping rate ($\gamma^{-1} = 25$) [3]. The observation of InAs plasmons could enable novel plasmonic circuits for future subwavelength applications.

[1] J. A. Schuller et al., Nat. Mater. 9, 193 (2010).
[2] D. K. Gramotnev et al., Nat. Photonics. 4, 83 (2010).
[3] Y. Zhou et al., Adv. Mater. 30, 1802551 (2018).

CPP 28: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge IV (joint session O/CPP/DS/TT)

Time: Tuesday 14:00–16:45 Location: H9

Topical Talk CPP 28.1 Tue 14:00 H9

The Data Revolution in Materials Science, Through the Lens of the Materials Project — •Kristin Persson — University of California, Berkeley, USA

Advanced materials are essential to economic and societal development, with applications in multiple industries, from clean energy, to national security, and human welfare. Historically, novel materials exploration has been slow and expensive, taking on average 18 years from concept to commercialization. Due to the tremendous improvements in computational resources, coupled with software development during the last decades, real materials properties can now be calculated from quantum mechanics much faster than they can be measured. A new era of computational materials prediction and design has been born. A result of this paradigm change are databases like the Materials Project which is harnessing the power of supercomputing together with state of the art quantum mechanical theory to compute the properties of all known inorganic materials and beyond, design novel materials and offer the data for free to the community together with online analysis and design algorithms. We leverage the rich data from the Materials Project for machine learning; accelerating materials design, characterization and finally synthesis of materials. This talk will survey this rapidly evolving and exciting paradigm in science, showcasing the possibilities and iteration between ideas, computations, insight and new materials development.

CPP 28.2 Tue 14:30 H9

High-throughput simulations of complex band structure — •Emanuele Bosoni and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2

The Complex Band Structure (CBS) generalizes the conventional band structure of a material by considering wave-vectors with complex components. The CBS extends the description of the allowed states of a material beyond the bulk propagating states, including in the picture the evanescent wave-functions that grow or decay from one unit cell to the next. Even though these latter states are forbidden by translational symmetry, they become important when this is broken via, for example, an interface. In the past, many studies made use of CBS calculations in order to confirm or motivate experimental findings, but only recently we see some efforts to give an unified prospective to the study of this quantity [1]. Moreover, the growth in recent years of high-performance computational resources available at relatively low cost opens the possibility to make a systematic, high-throughput, study of the CBS within the Density Functional Theory (DFT) framework.

In this contribution we will present our implementation of the Transfer Matrix Method [1] for the calculation of the CBS within the DFT code Siesta [2] and we will explain challenges and benefits of the high-throughput approach. We will present a proof of concept example in which we calculated the CBS for a set of materials and we will conclude explaining the relevance of our project in the field of spintronics.

[1] Reuter M. G., J. Phys.: Condens. Matt. 29, 053001 (2017)
[2] J. M. Soler et al., J. Phys.: Condens. Matt. 14, 2745 (2002)

CPP 28.3 Tue 14:45 H9

Computational Screening of 2D Materials for Solar Cells Application — •Anders Christian Riis-Jensen and Kristian Sommer Thygesen — Institute for Physics, Technical University of Denmark

Two-dimensional (2D) materials have attracted great attention in recent years, not least due to their extremely strong coupling to light and pronounced excitonic effects. This makes 2D materials an ideal playground for studying light-matter interaction in nano-scale materials for applications within e.g. solar cells and photo-detectors. In this work, we present a large-scale computational study of a wide variety of 2D materials with the aim of identifying novel candidates with strong light-matter interaction. Specifically, we calculate the absorption spectrum of almost 2000 materials at the level of the Random Phase Approximation (RPA) and/or by solving the Bethe-Salpeter Equation (BSE). This enables us of calculating the Power Conversion Efficieny (PCE) for all these materials fully ab-initio. Based on this we identify specific 2D semiconductors for both single- and tandem solar cells. The best candidates present power densities (PCE per unit mass) of several orders of magnitude larger than both Si and GaAs. Lastly, we also show a detailed analysis of a few 2D materials, in which we find exciton states with exceptionally strong coupling to light and large exciton binding energies.

CPP 28.4 Tue 15:00 H9

First-principles Modelling of Solid-Solid Interfaces in all Solid-State Batteries — •Bora Karasulu[1], James P. Darby[1], Clare P. Grey[2], and Andrew J. Morris[3] — [1]Dept. of Physics, Univ. of Cambridge, UK — [2]Dept. of Chemistry, Univ. of Cambridge, UK — [3]School of Metallurgy and Materials, Univ. of Birmingham, UK

All solid-state batteries (ASSBs) can potentially mitigate the safety issues known for conventional Li-ion batteries, and provide enhanced energy densities, by replacing the organic electrolyte solutions with solid inorganic equivalents. Mechanical and (electro)chemical incompatibilities between the ASSB solid components, however, lead to high resistances, curtailing the Li-ion transport at their interfaces. In this talk, we introduce a high-throughput ab initio modelling approach towards the rational design of electrolyte/electrode interfaces in ASSBs. First, we obtain phase diagrams of sulfide-based electrolytes with diverse compositions, phases, vacancies and doping using the Ab Initio Random Structure Searching (AIRSS) method. Next, the stable and low-lying metastable phases are screened for their ionic conductivity using ab initio molecular dynamics simulations. Finally, diverse surfaces of the selected electrolyte phases are interfaced with the surfaces of electrodes or other interfacial (e.g. solid electrolyte interphase, SEI) layers to determine the stable combinations using an automated procedure (INTERFACER). The devised approach will be demonstrated in action for a collection of interfaces, e.g. Li-P-S electrolytes with LiCo2, Li-metal electrodes and alike.

CPP 28.5 Tue 15:15 H9

New Insights into Amorphous Materials and their Surfaces by Combining Machine Learning and DFT — •Volker Deringer — University of Cambridge, Cambridge, UK

Understanding links between atomic structure, chemical reactivity, and physical properties in amorphous solids is a long-standing challenge. DFT-based atomistic simulations have played important roles in this, but come at high computational cost. Novel interatomic potentials based on machine learning (ML) achieve close-to DFT accuracy, but require only a small fraction of the cost. In this talk, I will argue that such ML-based potentials are particularly useful for studying amorphous solids.

First, I will describe a Gaussian Approximation Potential (GAP) for amorphous carbon, which we recently used to simulate the deposition of tetrahedral amorphous carbon (*ta*-C) films, one atom at a time. These simulations reproduced the experimentally observed count of sp^3 atoms and gave new insight into the microscopic growth mechanism. I will then discuss how ML-based potentials can be combined with density-functional methods to yield new insights into surface functionalization (specifically, hydrogenation and oxidation) of *ta*-C. Finally, I will present recent work on amorphous silicon, another prototypical non-crystalline material that ML-driven simulations can describe with high accuracy. Looking ahead, these studies suggest that ML-based potentials may become more widespread tools for the realistic modelling and understanding of the amorphous state.

CPP 28.6 Tue 15:30 H9

Harvesting from unbiased sampling of open systems: phase diagrams and property maps of surfaces and clusters in reactive atmosphere — •Yuanyuan Zhou, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Numerous processes that occur at surfaces of materials play a critical role in the manufacture and performance of functional materials, e.g., electronic, magnetic, and optical devices, sensors, catalysts, and coatings. A prerequisite for analyzing and understanding the electronic properties and the function of surfaces is detailed knowledge of the atomic structure, i.e., the surface composition and geometry under realistic condition. We introduce a Replica-Exchange (RE) Grand-Canonical (GC) Monte-Carlo algorithm. By means of the coupled sampling at several chemical potentials (i.e., partial pressures) of a reactive gas atmosphere and temperatures, the REGC scheme enables the unbiased calculation of (p, T) phase diagrams of surfaces, nanoparticles, or clusters in contact with reactive atmosphere, where all anharmonic contributions are included. Moreover, the multi-canonical sampling yields the temperature-pressure dependence (map) of all equilibrium observables that can be measured within the given model Hamiltonian. For instance, structural parameters such as the radial distribution function, or the fundamental electronic gap. This allows for rational design, where *operando* condition are taking fully into account. We demonstrate the approach for model Lennard-Jones surfaces as well as Si clusters and surfaces in a hydrogen atmosphere.

CPP 28.7 Tue 15:45 H9

Crystal structure prediction for high capacity battery materials — •Angela F Harper[1] and Andrew J Morris[2] — [1]Department of Physics, University of Cambridge, JJ Thomson Ave, Cambridge CB3 0HE, UK — [2]School of Metallurgy and Materials, University of Birmingham, Edgbaston, Birmingham, UK

The future of large-scale energy storage relies heavily on the ability of Li-ion batteries to have high capacity and long-term stability. At present, graphite anodes limit the overall capacity of Li-ion batteries to a theoretical maximum of 372 mAh/g, and thus there is a need for higher capacity anodes such as phosphorus. We have studied lithiation in phosphorus using a combination of *ab initio* random structure searching (AIRSS) and density-functional theory calculations. In the Li-P system we found a novel phase of $P2_12_12_1$ Li_4P_3, which showed stable 0K phonon modes [1]. We further showed, using defect AIRSS searches, that doping the known Li-P phases with aluminium improved their electronic density of states at the Fermi level, and could improve conductivity in phosphorus anodes. To improve the cyclability of these phosphorus anodes, which break down after several cycles due to volume expansion of over 200%, in this talk we will investigate the phase diagrams and voltage profiles of several ternary compounds of Li-P-M where M is a metallic element which maintains the conductivity of aluminium doping and adds stability to the anode.

[1] Mayo, M. et al. Chem. Mater. 2016, 28, 2011*2021

CPP 28.8 Tue 16:00 H9

Constructing Accurate Machine Learning Force Fields for Flexible Molecules — •Valentin Vassilev-Galindo, Igor Poltavsky, and Alexandre Tkatchenko — Physics and Material Science Research Unit, University of Luxembourg, Luxembourg

State-of-the-art machine learning (ML) models can reproduce potential energy surfaces (PES) for molecules containing up to a few tens of atoms with the accuracy comparable to the most exact ab initio methods. This provides a unique tool for computing different thermodynamic properties that would require millions of CPU years otherwise. For instance, a recently developed sGDML[1,2] model predicts forces and energy with CCSD(T) accuracy using just a few hundreds of configurations for training. However, up to now ML has been mainly applied to rather rigid molecules. In this regard, our objective is to test ML for flexible molecules and out-of-equilibrium configurations along transition paths. For this, we select molecules (e.g. azobenzene, stilbene) with relatively complex transition paths, which result from an interplay between long- and short-range interactions. Then, different paths connecting PES minima are tested using sGDML. This allows us to define optimal descriptors and the most appropriate strategies for choosing the training sets, which is crucial for ML models relying on a limited number of training points. Our results open an avenue for efficiently calculating transport pathways, transition rates and other out-of-equilibrium properties with previously unattended accuracy.

[1] Chmiela, S. et al., Sci. Adv. 3, e1603015 (2017).

[2] Chmiela, S. et al., Nat. Commun. 9, 3887 (2018).

CPP 28.9 Tue 16:15 H9

Calculating critical temperatures for magnetic order in two-dimensional materials — •Daniele Torelli — CAMD, Department of Physics, Technical University of Denmark, 2820 Kgs. Lyngby, Denmark

Recent observation of ferromagnetic out-of-plane order in two-dimensional (2D) CrI_3 highlights the importance of a microscopic understanding of magnetic anisotropy (MA) in ground state magnetic systems. Single-ion anisotropy and anisotropic exchange coupling comprise crucial ingredients to escape the Mermin-Wagner theorem which implies that rotational symmetry cannot be spontaneously broken at any finite temperature in 2D and thus prevents magnetic order.

In the present work we investigate the variation of critical temperature in Heisenberg model systems using classical Metropolis Monte Carlo simulations. A fit for square, hexagonal and honeycomb lattices leads to a simple expression for the critical temperatures as a function of MA and exchange coupling constants.

Based on a new developed computational 2D materials database, we predict 2D structures with high critical temperatures and high thermodynamic and dynamic stability for future experimental investigations. As testing system, relevant Heisenberg exchange couplings and MA energies in mono-layer CrI_3 are obtained from first principle calculations and energy mapping analysis, yielding to an estimation of Curie temperature in good agreement with experimental results.

CPP 28.10 Tue 16:30 H9

Amino-acids on metallic surfaces: searching conformational space — •Dmitrii Maksimov, Carsten Baldauf, and Mariana Rossi — Fritz-Haber-Institut der Max-Planck- Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Organic-inorganic interfaces are challenging for computational modeling, in particular regarding the prediction of stable configurations at the interface, which determine the electronic properties of the system as a whole. The amino acid arginine is a flexible molecule in the gas phase and experiments show its self-assembly into dimers, rings, and chains on Ag(111) and Au(111) surfaces. For two protonation states (neutral Arg and charged $ArgH^+$), we perform systematic structure searches by placing known gas-phase minima in different orientations on top of the surfaces, followed by full relaxation within long-range dispersion corrected density-functional theory (DFT). In the analysis, we aim at understanding the alterations of the conformational space from the gas phase to surface adsorption by means of a dimensionality-reduced representation based on a combination of the Smooth Overlap of Atomic Positions (SOAP) and the Sketchmap techniques [1]. The favorable interaction with the metallic surface reduces the number of accessible conformations for neutral Arg. For the adsorption of charged ArgH$^+$, the number of local minima increases due to surface-dependent partial charge screening. [1] S. De et al., *J. Cheminform.*, **9**:6 (2017)

CPP 29: Two-dimensional Materials II: graphene (joint session HL/CPP)

Time: Tuesday 14:00–15:45 Location: H36

CPP 29.1 Tue 14:00 H36

Field-controllable spin relaxation anisotropy in graphene/hBN heterostructures — •Klaus Zollner[1], Martin Gmitra[2], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute of Physics, P. J. Šafárik University in Košice, 04001 Košice, Slovakia

Measurements show a large and tunable anisotropy in the spin relaxation of hBN encapsulated bilayer graphene [1,2], similar to what is observed in graphene/TMDC heterostructures [3]. Combining systematic first principles calculations for graphene/hBN heterostructures with a minimal tight-binding model, we extract spin-orbit coupling parameters of graphene in the μeV range. The extracted model parameters depend on (i) interlayer distances, (ii) stacking configurations, and (iii) an external electric field, resulting in a rich parameter space. Based on the Dyakonov-Perel formalism we calculate spin relaxation times for graphene, in the nanosecond range, in agreement with recent experimental measurements. A very important finding is that the spin relaxation anisotropy is maximum close to the charge neutrality point, decreasing with the doping level. In addition, we also show that the anisotropy can be tuned by means of an external electric field, via the precise control of the Rashba SOC.

This work is supported by the DFG SPP 1666.

[1] Xu et al., PRL 121, 127703 (2018)

[2] Leutenantsmeyer et al., PRL 121, 127702 (2018)

[3] Cummings et al., PRL 119, 206601 (2017)

CPP 29.2 Tue 14:15 H36

Microscopic theory of band gap opening and spin-orbit splitting in graphene/TMDC heterobilayers — •Alessandro David[1], Andor Kormányos[2], and Guido Burkad[1] — [1]Department of Physics, University of Konstanz, Konstanz, Germany — [2]Department of Physics of Complex Systems, Eötvös Loránd University, Budapest, Hungary

Bilayers of graphene and monolayer transition metal dichalcogenides (TMDCs) are fascinating van der Waals heterostructures with an interesting electronic band structure. Theoretical ab initio calculations have shown a gap opening and a spin-orbit splitting in the band structure of graphene that are induced by the TMDC layer [1, 2]. These results have been experimentally confirmed by recent magnetotransport experiments showing weak antilocalisation (WAL) [2, 3]. Using perturbation theory, we propose a microscopic model to explain the origin of the gap and of the spin-orbit splitting. We also consider the dependence of the spin-orbit splitting on the misalignment of graphene and TMDC layers.

[1] M. Gmitra, D. Kochan, P. Högl, and J. Fabian, Phys. Rev. B 93, 155104 (2016). [2] Z. Wang, D.-K. Ki, H. Chen, H. Berger, A. H. MacDonald, and A. F. Morpurgo, Nat. Comm. 6, 8339 (2015). [3] T. Wakamura, F. Reale, P. Palczynski, S. Guéron, C. Mattevi, and H. Bouchiat, Phys. Rev. Lett. 120, 106802 (2018).

CPP 29.3 Tue 14:30 H36

Spatio-temporal dynamics in graphene — •Roland Jago, Samuel Brem, and Ermin Malic — Chalmers University of Technology, Gothenburg, Sweden

While the time- and energy resolved non-equilbirium dynamics in graphene is well understood [1], there is only little known about spatio-temporal electron dynamics. Optically excited carriers at the interfaces of inhomogeneities (e.g. p-n junctions, different substrate regions) create density and temperature gradients resulting in diffusion of carriers. Since many-particle interactions and diffusion depend on the conditions of the inhomogeneity, the transport of carriers is asymmetric and results in a photocurrent.

In this work, we apply the density matrix formalism solving the spatio-temporal graphene Bloch equations. We provide microscopic access to time-, momentum and spatially resolved optical excitation, Coulomb- and phonon-induced relaxation dynamics, and conversion of light into electrical current in graphene. The gained microscopic insights allow us to predict optimal conditions for photodetection in graphene.

[1] E. Malic and A. Knorr, Ultrafast optics and relaxation dynamics, VCH-Wiley, Berlin (2013)

CPP 29.4 Tue 14:45 H36

How Laser-induced defects modify optical properties of semiconducting Armchair Graphene Nanoribbons — •Seyed Khalil Alavi[1,2], Boris V. Senkovskiy[3], Markus Pfeiffer[1], Danny Haberer[4], Felix R. Fischer[4], Alexander Grüneis[3], and Klas Lindfors[1] — [1]Department of Chemistry, Universität zu Köln, Luxemburger Str. 116, 50939 Köln, Germany — [2]Institut für Angewandte Physik der Universität Bonn, Wegeler Strasse 8, 53115 Bonn, Germany — [3]II. Physikalisches Institut, Universität zu Köln, Zülpicher Strasse 77, 50937 Köln, Germany — [4]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Armchair graphene nanoribbons (AGNRs) with tunable band gap are promising candidate for optoelectronic devices. We have earlier shown how photoluminescence emission is boosted via formation of laser-induced defects in AGNRs lattices [1]. Here we probe the origin of this modification by measuring the extinction spectrum of a layer of AGNRs. Our results show that there are two pronounced peaks at approximately 2.4 and 1.8 eV in the spectrum of pristine GNRs. The latter peak energetically coincides with emission feature. This peak surprisingly disappears from the extinction spectrum after defects formation. We thus attribute the 1.8 eV peak to a quenching state. We additionally extract the absolute absorbance of AGNRs and find that it is a factor of three higher than graphene absorbance in visible range. [1] B. V. Senkovskiy, M. Pfeiffer, S. K. Alavi, et al., Nano Lett. 17, 4029-4037, 2017.

CPP 29.5 Tue 15:00 H36

Anisotropic strain induces a transition between rhombohedral and Bernal stacking in multilayer graphene flakes — Fabian Geisenhof[1], Raúl Guerro-Aviles[2], Marta Pelc[2], Felix Winterer[1], Tobias Gokus[3], Yasin Durmaz[3,4], Daniela Priesack[1], Jakob Lenz[1], Fritz Keilmann[4,5], Andres Ayuela[2], and •Thomas Weitz[1,4,5,6] — [1]AG Physics of Nanosystems, Faculty of Physics, LMU München, Germany — [2]Donostia International Physics Center, San Sebastian, Spain — [3]Neaspec GmbH, München, Germany — [4]Department of Physics, LMU München, Germany — [5]Center for Nanoscience (CeNS), München, Germany — [6]Nanosystems Initiative Munich (NIM), München, Germany

Graphene multilayers are still full of surprises - this is clear at latest since the recent discovery of unconventional superconductivity in 'magic-angle' bilayer graphene. Not only in bilayers the density of states critically depends on the lateral alignment of subsequent layers, but also in thicker graphene stacks (e.g. in trilayers). There, two different forms of stacking, so called Bernal and rhombohedral stacking exist, each with distinct charge transport properties. Via combined theoretical and experimental efforts we have surprisingly found [1], that during the fabrication process with conventional e-beam lithography, anisotropic strain forces rhombohedrally stacked regions towards Bernal stacking. We have experimentally identified the stacking change with Raman spectroscopy and s-SNOM measurements and devised methods how to avoid the transformation. [1] F.G. Geisenhof et al. ArXiv:1810.00067 (2018)

CPP 29.6 Tue 15:15 H36

Bio-compatible graphene exfoliation assisted by flavin mononucleotide sodium: a molecular dynamics study — •Shirong Huang[1], Alexander Croy[1], Viktor Bezugly[1,2], and Gianaurelio Cuniberti[1,3] — [1]Institute for Materials Science and Max Bergmann Center for Biomaterials, Technische Universität Dresden, 01062 Dresden, Germany — [2]Life Science Inkubator Sachsen

GmbH & Co. KG, Tatzberg 47, 01307 Dresden, Germany — [3]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, German

Flavin mononucleotide sodium (FMNS) was reported as a highly efficient bio-dispersant for the exfoliation of aqueous dispersions of defect-free, few-layer graphene flakes. Most importantly, FMNS is innocuous and environment friendly and can facilitate bio-medical applications of graphene. Although there is some experimental work on graphene exfoliation assisted by FMNS, it is not clear how FMNS molecules behave on the graphene flake. Here, we clarify the interaction between FMNS and graphene flakes via all-atom molecular dynamic simulations. The exfoliation mechanism of FMNS on the graphene flake is investigated by the potential of mean force (PMF) of pairs of graphene flakes coated with FMNS. This work provides a basis for understanding of graphene exfoliation assisted by FMNS-like surfactants and paves a path to design highly efficient dispersants for defect-free, few layer graphene.

CPP 29.7 Tue 15:30 H36

Scanning Nitrogen-Vacancy Center Magnetic Imaging of Graphene Devices — •Susanne Baumann, Alec Jenkins, Simon Meynell, Haoxin Zhou, Andrea Young, and Ania Bleszynski Jayich — UC Santa Barbara, Santa Barbara, USA

The NV center is a quantum probe that is sensitive to a variety of fields (magnetic, electric, thermal, strain), can achieve nanoscale spatial resolution, is non-invasive, and can operate over a wide range of temperatures; hence it is an ideal tool for studying novel phases of matter that often emerge only below a critical temperature. Here we use a cryogenic scanning NV magnetometer to probe the stray magnetic field of a current running through a single layer graphene device. With this technique we are able to probe different regimes of current flow via their local signatures over a variety of temperatures.

CPP 30: Complex Fluids and Colloids, Micelles and Vesicles (joint session CPP/DY)

Time: Wednesday 9:30–12:45 Location: H14

Invited Talk CPP 30.1 Wed 9:30 H14

Microstructural transitions and characterization of capillary suspensions — Sebastian Bindgen[1], Frank Bossler[2], Irene Natalia[1], and •Erin Koos[1] — [1]Department of Chemical Engineering, KU Leuven, Leuven, 3001, Belgium — [2]Institute for Mechanical Process Engineering, Karlsruhe Institute of Technology, Gotthard-Franz-Str. 3, 76131 Karlsruhe, Germany.

Suspensions can exhibit a wide range of rheological behaviors that are closely linked to both the bulk particle structure as well as the microstructure including direct particle contacts. Graph theory offers methods and parameters that can be used to analyze complex structures. This method is demonstrated using ternary liquid-liquid-solid systems, which exhibit a wide variety of different morphologies depending on the ratio of the three components. We analyze these networks using the coordination number and clustering coefficient. These parameters are compared to the measured storage and loss moduli.

These capillary suspension networks also exhibit atypical rheological behavior. For instance, a negative normal stress difference is observed from re-orientation of the flocs into the vorticity direction during shearing. Typically, systems with negative normal stress differences have either high volume concentrations and are shear thinning, or are shear thickening with very low particle concentrations. In contrast, the capillary suspensions we report here have a 25% solid concentration and are shear thinning; a combination that has never before been reported in literature.

CPP 30.2 Wed 10:00 H14

Flow of silica rods in microfluidic channels — •Hansol Jeon[1] and Dirk Aarts[2] — [1]Max Planck Institute for dynamics and self-organization, Göttingen, Germany — [2]University of Oxford, Oxford, United Kingdom

This project presents the flow of dense liquid crystal phases of colloidal silica rods in microfluidic channels. We describe the synthesis of silica rods that exhibit three different phases (isotropic, nematic and smectic). Using microfluidic channels of novel designs, we observe the flow behaviour of silica rods in the channels by confocal microscopy. We then conduct image analysis to track the dyed rods and measure the flow profile. We compare the flow profiles with the theory and provide future outlook to this experiment.

CPP 30.3 Wed 10:15 H14

Dynamics during the formation of an arrested protein phase separation studied using X-ray photon correlation spectroscopy — •Nafisa Begam[1], Anita Girelli[1], Anastasia Ragulskaya[1], Hendrik Rahmann[2], Kevin Lopata[2], Fabian Westermeier[3], Christian Gutt[2], Fajun Zhang[1], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Universität Siegen, Germany — [3]Petra III, DESY, Germany

Phase separation in aqueous protein solutions is of primary interest in the field of many biological and chemical processes. It is observed that the glass line often interrupts the phase separation [1] and leads the solution to a dynamically arrested state which results in a drastic reduction of the microscopic relaxation rate. Kinetics of phase separation of such a system of bovine γ-globulin in the presence of polyethylene glycol studied using ultra-small angle X-ray scattering [2] shows an arrest for a quench to temperatures below $\sim 2.5°$C. Here, our goal is to study the dynamics of the solution while approaching such an arrested state. We have used X-ray photon correlation spectroscopy which provides the time evolution of dynamics in the form of two time correlation (TTC) functions. A systematic study of the evolving dynamics of protein solutions during arrest at different quench temperatures using TTC exhibits initially an exponential growth of the relaxation time and at the later stage, an ageing heterogeneous dynamics. This study reveals a comprehensive picture of the protein dynamics that leads the solution to an arrested state. [1] Cardinaux et. al, *Phys. Rev. Lett.*, **99**, 118301, (2007) [2] S. Da Vela et. al, *Soft Matter*, **13**, 8756, (2017)

CPP 30.4 Wed 10:30 H14

Electron-Atom duality in DNA-programmable assembly — •Martin Girard[1], Anindita Das[2,4], Shunzhi Wang[2,4], Jingshan Du[3,4], Byeongdu Lee[5], Chad A. Mirkin[2,4], and Monica Olvera de la Cruz[3,6] — [1]Max Planck Institute for Polymer Physics, Mainz, Germany — [2]Department of Chemistry, Northwestern University, Evanston, IL, USA — [3]Department of Material Science and Engineering, Northwestern University, IL, USA — [4]International Institute for Nanotechnology, Evanston, IL, USA — [5]X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, IL, USA — [6]Department of Physics and Astronomy, Northwestern University, Evanston, IL, USA

A powerful method for designing colloidal crystals involves the use of DNA as a particle-directing ligand. With such systems, DNA-nanoparticle conjugates are considered programmable atom equivalents (PAEs), and design rules have been devised to engineer complex crystallization outcomes. Here, we report a new property of PAEs, a type of electron-atom duality. When reduced in size and DNA grafting density, PAEs can behave as electron equivalents (EEs) and move through lattices defined by larger PAEs. In such mixtures, the EEs roam through the crystals as electrons do in metals, holding the large PAEs in specific lattice sites. As the number of strands increases or the temperature decreases, the EEs localize yielding a transition from a metal to a compound. This concept of electron-atom-equivalent duality changes the way we think about colloidal systems and helps define new routes to metallic, intermetallic, and compound phases.

CPP 30.5 Wed 10:45 H14

Interaction forces in model cement systems — •Simon Becker and Regine von Klitzing — Soft Matter at Interfaces, Institut für Festkörperphysik, TU Darmstadt

For the workability of concrete and cement as highly abundant construction materials the flow behaviour in the early stages of these materials is of special interest. This can be influenced using additives such as super plasticizers to decrease the viscosity of cement pastes, yielding an enhanced workability. A better understanding of the interactions on the nanoscopic level and the impact on the macroscopic rheology is of great importance in the development of higher performing additives.

The interaction between model particles is mapped via colloidal-probe atomic force microscopy (CP-AFM) in sphere-sphere geometry. Combining CP-AFM with optical microscopy allows to arrange colloidal particles coaxially and determine the interaction forces between these particles upon approach. Spherical silica beads with diameters in the micrometer range serve as model cement grains due to the restriction of the AFM technique to either spherical particles or particles with a defined roughness. The influence on the interaction forces of these model grains in presence of different pH and different salts such as KCl and $CaCl_2$ and their concentrations is investigated. Furthermore the change of the interaction between the model particles in presence of different concentrations of PCE is examined.

CPP 30.6 Wed 11:00 H14

Computing the 3D Radial Distribution Function from Particle Positions: An Advanced Analytic Approach — •Bernd F. A. Kopera and Markus Retsch — Department of Chemistry, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth

The radial distribution function, g(r), is ubiquitously used to analyze the internal structure of particulate systems. However, experimentally derived particle coordinates are always confined to a finite sample volume. This poses a particular challenge on computing g(r): Once the radial distance, r, extends beyond the sample boundaries in at least one dimension, substantial deviations from the true g(r) function can occur. State of the art algorithms for g(r) mitigate this issue for instance by using artificial periodic boundary conditions. However, ignoring the finite nature of the sample volume distorts g(r) significantly. Here, we present a simple, analytic algorithm for the computation of g(r) in finite samples. No additional assumptions about the sample are required. The key idea is to use an analytic solution for the intersection volume between a spherical shell and the sample volume. In addition, we discovered a natural upper bound for the radial distance that only depends on sample size and shape. This analytic approach will prove to be invaluable for the quantitative analysis of the increasing amount of experimentally derived tomography data.

15 min. break

CPP 30.7 Wed 11:30 H14

A classical density functional from machine learning and a convolutional neural network — •shangchun Lin and Martin Oettel — Institut für Angewandte Physik, Universität Tübingen , Tübingen, Deutschland

We use machine learning methods to approximate a classical density functional. The functional *learns* by comparing the density profile it generates with that of simulations. As a study case, we choose the model problem of a Lennard Jones fluid in one dimension where there is no exact solution available and training data sets must be obtained from simulations. After separating the excess free energy functional into a "repulsive" and an "attractive" part, machine learning finds a functional in weighted density form for the attractive part. The density profile at a hard wall shows good agreement for thermodynamic conditions beyond the training set conditions. This also holds for the equation of state if it is evaluated near the training temperature.

CPP 30.8 Wed 11:45 H14

Semi-dilute mixtures of circular and linear polymers - towards novel separation techniques — •Lisa B. Weiss[1], Christos N. Likos[1], and Arash Nikoubashman[2] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna,Austria — [2]Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany

Linear polymers have been extensively studied in various concentration regimes, at rest and when exposed to a variety of flow fields. Recently, this interest extended to ring polymers, focusing on melts and dilute solutions. When diluted and at rest, rings show the same scaling behavior as chains, but when exposed to non-equilibrium conditions astonishing differences become apparent uniquely related to their topology. Furthermore, entangled rings show in equilibrium as well as when sheared marked differences compared to their linear counter part. However, the semi-dilute regime of pure ring polymer solutions and topological mixtures of rings and chains have been sparsely investigated so far. To resolve this, we simulate pure linear and ring polymer solutions and their mixtures around the overlap concentration at rest and under Hagen-Poiseuille flow. To correctly take into account hydrodynamic interactions, we employ the multi-particle collision algorithm. Mixtures of chains and rings show a distinct cross stream migration behavior at any investigated concentration, offering a promising route towards novel separation techniques. In particular, we observed a pronounced propensity of the rings to focus at the channel center while the chains populate the region close to the confining walls.

CPP 30.9 Wed 12:00 H14

Ring polymers in confined geometries with mixed boundary conditions — •Zoryana Usatenko[1], Piotr Kuterba[2], and Joanna Halun[3] — [1]Institute of Physics, Cracow University of Technology, Cracow 30-084, Poland — [2]Jagiellonian University, Cracow 30-348, Poland — [3]Institute of Nuclear Physics PAN, Cracow 31-342, Poland

Investigation of a dilute solution of phantom ideal ring polymers and ring polymers with excluded volume interactions in a good solvent confined in a slit geometry of two parallel walls with mixed boundary conditions which corresponds to the case of one repulsive and the other one inert wall is performed. Besides, taking into account the Derjaguin approximation the investigation of a dilute solution of ring polymers confined in a solution of mesoscopic colloidal particles of big size with different radii and different adsorbing or repelling properties in respect for polymers is performed. The calculation of the dimensionless depletion interaction potentials, the depletion forces and the monomer density profiles were performed in the framework of the massive field theory approach at fixed space dimension $d<4$ up to one loop order. The density-force relation in the case of phantom ideal ring polymer chains is analyzed and the respective universal amplitude ratio is calculated. The obtained results indicate the interesting and nontrivial behaviour of ring polymers in confined geometries and give possibility better to understand the complexity of physical effects arising from confinement and chain topology, especially in the case of interaction of λ bacteriophages with E.coli bacteria cells.

CPP 30.10 Wed 12:15 H14

Multi-scale simulations of polymeric nanoparticle fabrication through rapid solvent exchange — •Arash Nikoubashman[1], Nannan Li[2], and Athanassios Panagiotopoulos[2] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz, Mainz, Deutschland — [2]Department of Chemical and Biological Engineering, Princeton University, Princeton, USA

Tailored nanoparticles are increasingly sought after for many scientific and technological applications, such as optoelectronic devices and selective catalysts. However, both research and commercialization of these materials has been impeded by the lack of suitable fabrication techniques. One promising approach for overcoming this hurdle is flash nanoprecipitation, where (soft) nanoparticles are assembled through rapid micromixing of polymers in solution with a miscible poor solvent. This continuous process allows for high yields as well as precise control over particle size and morphology. We employed multiscale simulations of this process to understand its underlying mechanisms and to efficiently explore parameter space. We first performed explicit solvent molecular dynamics (MD) simulations of a bead-spring polymer model to study the microscopic properties of the fabrication process. Then, we fed the MD data into a kinetic Monte Carlo algorithm to reach macroscopic length- and timescales. We discovered that the nanoparticle size can be reliably tuned through the initial polymer concentration and the mixing rate. Further, we were able to fabricate a wide variety of structured colloids, such as Janus and core-shell particles, when polymer blends were used in the feed stream.

CPP 30.11 Wed 12:30 H14

Molecular Simulation of Thermodynamic Properties with the Osmotic Equilibrium Approach: Accessing Activities in Complex Concentrated Liquid Phases — •Michael Bley[1,2], Magali Duvail[1], Philippe Guilbaud[3], and Jean-François Dufrêche[1] — [1]ICSM, CEA, CNRS, ENSCM, Univ Montpellier, BP 17171, F-30207 Bagnols-sur-Cèze, France — [2]Applied Theoretical Physics-Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder Str. 3, D-79104 Freiburg, Germany — [3]Nuclear Energy Division, Research Department on Mining and Fuel Recycling Processes (SPDS/LILA), CEA, BP 17171, F-30207 Bagnols sur Cèze, France

Thermodynamic properties such as activities of complex concentrated liquid phases are a key parameter for describing chemical equilibria by means of mass action law. The mass action law and the corresponding equilibrium constant provide a measure for the direction of any chemical equilibrium. The osmotic equilibrium approach has been developed for accessing activities for a huge bandwidth of complex liquid systems.

Starting from Molecular Dynamics (MD) simulations of vapor-liquid interfaces using explicit polarization provides a direct access to the activity by comparing the mean amount of evaporated molecules of a given species in the vapor phase for a mixture and for the pure species, respectively. Obtained structures and thermodynamic properties showed a very good agreement with previous experimental and theoretical studies on various aqueous electrolyte solutions and organic solvent phases up to high solute concentrations.

CPP 31: Organic Electronics and Photovoltaics II - Non-Fullerene Organic Solar Cells

Time: Wednesday 9:30–11:00 Location: H18

CPP 31.1 Wed 9:30 H18

Loss Processes in Non-fullerene Acceptor Bulk Heterojunction Solar Cells — •Frédéric Laquai — King Abdullah University of Science and Technology, KAUST Solar Center, Thuwal, Saudi Arabia

Organic solar cells that use non-fullerene acceptors (NFA) are now outperforming their fullerene-based counterparts with efficiencies exceeding 14%. While the photophysics of fullerene-based systems have been studied quite intensively, the complex interplay between structure, morphology, photophysics, and efficiency of non-fullerene acceptor devices remains less well understood; yet, understanding the structure-property relations is an important prerequisite for a guided material design and further efficiency enhancements. In this contribution, I will discuss what currently limits the quantum efficiency in blends of common donor polymers and novel non-fullerene acceptors. By using steady-state and transient spectroscopy techniques and advanced data analysis tools, we are able to distinguish the spectral contributions and dynamics of singlet excitons, charge carriers, and triplet states and to quantify their concentration across a wide dynamic range relevant to the solar cell performance. Furthermore, we investigate how the CT-state energy, radiative, and non-radiative losses in non-fullerene acceptor blends influence the open-circuit voltage and we address the origin of low fill factors sometimes observed in NFA systems. This allows us to develop a precise picture of the efficiency-limiting processes in solar cells that use novel non-fullerene acceptors.

CPP 31.2 Wed 9:45 H18

Analysing geminate and non-geminate losses in high performance non-fullerene blends — •Lorena Perdigón-Toro[1], Huotian Zhang[2], Safa Shoaee[1], Feng Gao[2], and Dieter Neher[1] — [1]University of Potsdam, Institute of Physics and Astronomy, Germany — [2]Linköping University, Department of Physics, Chemistry and Biology (IFM), Sweden

Organic solar cells consist of blends of two or more semiconductors with different electronic structures, namely organic electron donors and acceptors. Recently, interest has increased towards non-fullerenes (NF) as the small-molecule acceptor. Organic cells benefit from the NF long wavelength absorption, which provides the blend with a broader coverage of the sun spectrum and thus, higher short-circuit currents. Moreover, devices containing NFs show high open-circuit voltages meaning that charge separation occurs efficiently even with small driving forces. In this work we study charge generation and recombination in a set of NF devices with efficiencies up to 13%. While all blends exhibit similar low voltage losses, the fill factors (FF) of the solar cells differ greatly, pointing to significant differences in geminate and/or non-geminate recombination. Time delayed collection field (TDCF) and bias assisted charge extraction (BACE) were used to disentangle these processes. Indeed, the devices with lower FF suffer from field-dependence of charge generation and faster bimolecular recombination. Altogether, the obtained recombination coefficients together with SCLC-measured mobilities allow reconstructing the FF, clearly pointing to these parameters as those to address for higher overall performance.

CPP 31.3 Wed 10:00 H18

Triplet Excitons in Non-Fullerene Acceptor-Polymer Blends and Organic Solar Cells? — •Maria Kotova, Johannes Junker, Andreas Baumann, Kristofer Tvingstedt, Andreas Sperlich, and Vladimir Dyakonov — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

In the past, most organic solar cells (OSCs) employed fullerenes as electron acceptors. Recently, the synthesis of novel non-fullerene acceptors (NFA) resulted in significantly higher power conversion efficiencies (PCE) of over 13%. It has been shown, that in fullerene-based OSCs the formation of triplet excitons (TE) opens an additional recombination pathway. In this work, the formation of TEs in NFA-based OSCs is investigated. We studied optical, electrical and spin properties of the polymer donor PBDB-T and the NFA acceptor ITIC in pristine films, in blend films and OSCs based on the blend. OSCs show a PCE of 9.8% and external quantum yield of up to 73%. Low temperature spin-sensitive photoluminescence measurements reveal the formation of highly localized TEs in pristine films of the donor (D) and acceptor (A), as well as in the blend films. This can occur either via intersystem crossing (ISC) or electron back transfer (EBT). ISC is likely for low mobility singlet excitons that cannot reach D-A interfaces and cannot dissociate into CT states. The EBT forms TE from the CT states. However, no TE signal was observed in solar cells under working conditions, thus no significant ISC or EBT occurs and the triplet formation loss channel is not very efficient. The lack of TEs matches well with the high PCE of NFA-based OSCs and their stability.

CPP 31.4 Wed 10:15 H18

Fullerene-free bulk heterojunction blends for photovoltaic applications - a morphological study — •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

In the last decades, organic electronics have been in the focus of research due to their advantageous properties, such as versatility, flexibility, low-cost manufacturing processes, like roll-to-roll printing or spray casting, and the tunable characteristics. These properties open up a wide range of applications and represent a promising alternative for the conventional inorganic photovoltaics. Even though the power conversion efficiency is lower than the ones of conventional devices, values of over 11% have been reported. Thereby, systems using low-band gap polymers and non-fullerene small molecules have received increasing attention. We study the inner morphology of such a bulk heterojunction blend, namely PBDB-T and ITIC of different compositions with grazing-incidence small-angle X-ray scattering (GISAXS). The obtained structural information are correlated with current density-voltage characteristics and the absorbance of the active layer in order to improve the efficiency.

CPP 31.5 Wed 10:30 H18

Long term UV stable organic solar cells by utilizing a stable donor-acceptor-additive combination — •Thomas Heumüller, Andrej Classen, Yakun He, Lukas Einsiedler, Johannes Gerner, Ning Li, and Christoph Brabec — Friedrich-Alexander-Universität Erlangen-Nürnberg

With the advent of non-fullerene acceptors (NFA), current state of the art organic solar cells (OSC) reach efficiencies around 14 % and an efficiency of 10 % is surpassed for plenty of systems. However, little is known about the stability and lifetime of current NFA based OSCs. Here we present a detailed degradation analysis of OSCs based on a polymer (PBQ-QF) which exhibits a good performance when blended with two different NFAs (ITIC and o-IDTBR) as well as PC70BM. In order 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 we focus on the degradation in dependence of UV light. Under full AM 1.5G light spectrum (1000 h continuous illumination) we observe an intense degradation of PBQ-QF:PC70BM while PBQ-QF:ITIC exhibits a moderate stability and PBQ-QF:o-IDTBR is highly stable. Interestingly we find, that the strong degradation of PBQ-QF:PC70BM can be lifted when UV cut-off filters are applied. The in-depth analysis reveals that the UV instability originates from a UV instability of PC70BM towards the processing additive 1,8 diiodooctane.

CPP 31.6 Wed 10:45 H18

Enthalpy of Charge Transfer Energetics for Organic Photovoltaics based on anthracene-containing PPE-PPVs and ITIC

— •Shahidul Alam[1,2], Christian Friebe[1,2], Johannes Ahner[2], Martin Hager[1,2], Daniel A. M. Egbe[3], Tomas Vary[4], Vojtech Nádaždy[4], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]FSU Jena, Germany — [2]IOMC, Jena, Germany — [3]JKU, Linz, Austria — [4]SUT, Bratislava, Slovak Republic

Lately, NFAs have received increasing attention for use in polymer-based bulk-heterojunction OPVs, as they have demonstrated improved PV performances over classical polymer-fullerene blends. Part of the success of these materials has to be attributed to a considerable contribution to the overall absorption of the solar cells, thanks to relatively low bandgaps in these materials. In this study a systematic comparison between two acceptor materials, the classical fullerene-derivative PCBM and the NFA ITIC was performed in combination with AnE-PVstat. The photo-induced charge transfer occurring at the D-A interface within an organic semiconductor (bulk) heterojunction is considered to be driven by the energy level offset between the corresponding LUMO of the same. Commonly, these energy offsets between LUMO levels of D-A are taken from CV characterization of organic semiconductors in film or solution. While the such derived energy levels seem to suggest successful charge transfer from the polymer to the ITIC, blend films and PV studies show the opposite. Literature, various spectroscopic, morphological and structural characterization methods have been used for finding an explanation.

CPP 32: Charged Soft Matter, Polyelectrolytes and Ionic Liquids I

Time: Wednesday 9:30–13:00 Location: H13

CPP 32.1 Wed 9:30 H13

Polyelectrolyte Multilayers from Binary Mixtures of Polyanions: Different Composition in Film and Solution — •Annekatrin Sill, Antonia Weltmeyer, Peter Nestler, Amir Azinfar, Malte Passvogel, and Christiane A. Helm — Universität Greifswald, Institut für Physik, Felix-Hausdorff-Str. 6, 17489 Greifswald

Polyelectrolyte multilayers were prepared from polyanion PSS and polycation PDADMA in 0.1 M NaCl. PSS consisted of binary mixtures of heavy deuterated PSSd (Mw(PSSd) = 80.8 kDa) and light protonated PSS (Mw(PSS) = 10.6 kDa). With neutron reflectivity, it was found that the film contained a larger mole fraction PSSd than the deposition solution. If the mole fraction ϕPSSd(80.8 kDa) in the deposition solution exceeded 5 %, the multilayer consisted only of heavy PSSd. The time-resolved adsorption was studied with in-situ ellipsometry. Each polycation deposition step was followed by partial desorption of the top layer which is attributed to desorption of PDADMA complexed by light PSS molecules. These studies show that the polymer composition in the adsorption solution and in the adsorbed multilayer may differ.

CPP 32.2 Wed 9:45 H13

Adsorption Behaviour of oppositely charged Polyelectrolyte/Surfactant Mixtures: Influence of Salt — •Larissa Braun and Regine von Klitzing — Department of Physics, TU Darmstadt, Darmstadt, Germany

The surface properties of oppositely charged polyelectrolyte/surfactant mixtures play an important role in colloidal dispersions (foams, emulsions) e.g. for cosmetics, cleaning products and in food technology. The present study addresses the influence of the ionic strength on the surface tension of polyanions (NaPSS or sPSO$_2$-220) mixed with cationic C$_{14}$TAB. Depending on the counterion of the polyanion LiBr or NaBr is used.

In case of NaPSS NaBr reduces the surface tension over the whole studied polyelectrolyte concentration range (10^{-5} * 10^{-3} monoM) and broadens the increase of surface tension at the bulk stoichiometric mixing point (BSMP) of polyelectrolyte and surfactant. In contrast, LiBr reduces the surface tension of sPSO$_2$-220 only above the BSMP.

These finding will be correlated the surface excesses and surface structure of the polyelectrolyte/surfactant mixtures obtained by neutron reflectometry measurements.

CPP 32.3 Wed 10:00 H13

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

Polymeric ionic liquids (PILs) combine the advantages of neat ionic liquids with the mechanical benefits of polymers, which gives rise to the importance of those materials in supercapacitors, battery media, or gas separator membranes. Even though extensive research has been conducted driven by interest on the devices' macroscopic performance, knowledge about molecular interactions is still not complete. Recently, it has been reported from a novel PIL which exhibits one of the highest values of DC-conductivity at temperatures below 100°C and – contrary to the common dogma – conductivity that does *not decrease* with rising degree of polymerization [F. Frenzel, R. Gutermann, A. M. Anton, J. Yuan, F. Kremer; *Macromolecules*, **50**, (2017), 4022 – 4029].

In order to characterize this material further a set of experiments adapted to study *inter-* as well as *intra-molecular* interactions is examined. Temperature-dependent FTIR spectroscopy reveals extensive hydrogen bonding of particular moieties, whereas other parts are effectively screened. Temperature- and frequency-dependent broadband dielectric spectroscopy (BDS) confirms reduced charge transport (26% reduction) in correlation with hydrogen bonding arising from hindered mobility. Moreover, in comparison to hydrogen bonding the influence of temperature-activated molecular mobility on the conductivity is considerably stronger ($\approx$ 3 orders of magnitude).

CPP 32.4 Wed 10:15 H13

Competing interactions and the formation of dynamic protein clusters — •Anita Girelli[1], Michal K. Braun[1], Alessandro Marianini[2], Fajun Zhang[1], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]ESRF Grenoble, France

Controlling of cluster formation is of high relevance in biology, biomedicine and pharmacy. In this study solutions of bovine serum albumin with LaCl$_3$ were studied using small angle x-ray scattering (SAXS) and dynamic light scattering (DLS) to characterize the static and dynamic properties of protein clusters. The system has a reentrant phase behavior [1], before the system enters the condensation regime the presence of long range repulsion and short range attraction leads to the cluster formation [2]. DLS and SAXS data suggest the formation of clusters for a ratio of salt and protein concentration $c_s/c_p > 3$, supported also by neutron backscattering experiments [3]. The SAXS data for samples with a series of concentrations were fitted with a law $q_c = a\phi^b$, where ϕ is the volume fraction and q_c the position of the correlation peak present in the structure factor. The parameter b was found to have a value larger than 1/3. Based on geometrical consideration this suggest that the number of clusters decreases for increasing protein concentration. This could be attributed to an entropic effect or to an increase of ionic strength.

[1] Zhang et al., *Phys. Rev. Lett.*, **101**, 148101, 2008
[2] D. Soraruf et al., *Soft Matter*, **10**, 894, 2014
[3] Grimaldo et al., *J. Phys. Chem. Lett.*, **6**, 2577, 2015

CPP 32.5 Wed 10:30 H13

Phase separation kinetics in protein-salt mixtures with compositionally tuned interactions — •Olga Matsarskaia[1], Stefano Da Vela[1], Alessandro Mariani[2], Zhendong Fu[3], Fajun Zhang[1], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]ESRF, Grenoble, France — [3]JCNS@MLZ, Garching, Germany

Liquid-liquid phase separation (LLPS) in protein systems is relevant for phenomena such as protein condensation diseases, subcellular organisation or protein crystallisation. Understanding and controlling LLPS in proteins is therefore crucial for a number of research areas. Bovine serum albumin (BSA) has been shown to have a lower critical solution temperature-LLPS (LCST-LLPS) induceable by multivalent salts. Importantly, the nature of the employed multivalent cations influences this LCST-LLPS. Here, we present a systematic ultra-small angle X-ray scattering (USAXS) investigation of the kinetics of LCST-LLPS of BSA in the presence of different ratios of HoCl$_3$ and LaCl$_3$, resulting in different effective overall attraction strengths. We monitor the characteristic length scales $\xi(t, T_{fin})$ after inducing LLPS by subjecting the respective systems to temperature jumps into their liquid-

liquid coexistence regions. With increasing interprotein attraction and increasing T_{fin}, we observe an increasing deviation from the growth law of $\xi \sim t^{1/3}$ and an increased trend towards arrest despite the fact that all the cations employed are nominally trivalent. We thus establish a method for fine-tuning phase transitions in our systems with several control parameters. Our findings help shed light on general aspects of protein LLPS and its tunability.

CPP 32.6 Wed 10:45 H13

Competition among metal cations for RNA binding: Results beyond Poisson-Boltzmann theory — •Sergio Cruz-León and Nadine Schwierz — Department of Theoretical Biophysics, Max Planck Institute of Biophysics, Max-von-Laue-Str. 3, 60438 Frankfurt, Germany.

The negative charge of RNA in solution alters the local ionic environment. An accurate modeling of the ionic atmosphere is therefore essential to correctly describe RNA stability, folding or association. In this work, we combine the result from all-atom molecular dynamics simulations with Poisson-Boltzmann theory. Our modeling allows us to capture the microscopic cation-RNA interactions, and to directly compare to ion counting (IC) experiments. For monovalent cations, the experimental competition constants are reproduced without further adjustments. For divalent metal cations, our results indicate that the current atomistic force field for Mg2+ ions overtimes the binding affinity. After optimization the Mg2+ force field based on experimental binding affinity, the experimental IC results can be reproduced without any fitting parameters. Therefore, combining molecular dynamics simulation with optimized ionic force fields and Poisson-Boltzmann theory allows us to gain microscopic insight into the ionic atmosphere and reproduce IC experiments with higher accuracy compared to previous theoretical models.

CPP 32.7 Wed 11:00 H13

Kinetic Pathways of Water Exchange in the First Hydration Shell of Magnesium — •Nadine Schwierz — Max Planck Institute of Biophysics

Water exchange between coordination shells of metal cations in aqueous solutions is fundamental in understanding the reactivity of the ions and their binding kinetics. Simulating water exchange with atomistic resolution is challenging due to the broad range of timescales involved ranging from picoseconds to milliseconds. Here, we apply a combination of transition path sampling and Umbrella sampling to accurately determine the exchange rates and to gain atomistic insight into the molecular pathways of water exchange. Using a recently developed atomistic model for Magnesium, water molecules remain in the first hydration shell for 10 ms on average, a time considerably longer compared to the 0.1 ms predicted by transition state theory using a single ion-water distance as order parameter. The discrepancy between these time scales arises from neglected degrees of freedom of other solvent molecules which play a decisive role in the reaction mechanism of water exchange.

15 min. break

CPP 32.8 Wed 11:30 H13

Specific ion effects for polyelectrolytes in aqueous and non-aqueous media: the importance of the ion solvation behavior — Anand Narayanan Krishnamoorthy[1], Christian Holm[1], and •Jens Smiatek[1,2] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Helmholtz-Institute Münster: Ionics in Energy Storage (HIMS - IEK 12), Forschungszentrum Jülich, Germany

We present the results of atomistic molecular dynamics simulations regarding specific ion effects in water, methanol and N,N-dimethylacetamide (DMAc). As reference system, we introduce rigid and rod-like models of polyanions and polycations in combination with alkali metal cations and halide anions as counterions. Pronounced specific ion effects can be observed in terms of the individual anion and cation condensation behavior. The outcomes of our simulations thus reveal significant differences to standard electrostatic mean-field theories. A detailed investigation of the individual energy contributions shows that ion-dipole interactions play a pivotal role in order to rationalize the findings. The corresponding deviations in terms of the cation and anion distribution can be brought into agreement with the donor and acceptor numbers of the solvents, which thus highlight the importance of solvent-ion interactions in addition to electrostatic attraction.

CPP 32.9 Wed 11:45 H13

A combined computational and experimental study on the microscopic structures in aqueous ionic liquids near solid/liquid and air/liquid interfaces — •Takeshi Kobayashi[1], Andre Kemna[2], Björn Braunschweig[2], Maria Fyta[1], and Jens Smiatek[1,3] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Institute of Physical Chemistry and Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany — [3]Helmholtz-Institute Münster: Ionics in Energy Storage (HIMS - IEK 12), Forschungszentrum Jülich, Corrensstraße 46, 48149 Münster, Germany

Even small amounts of water molecules may limit the use of common hygroscopic ionic liquids (ILs) as electrolyte solutions in electrochemical cells. Similar concentration-dependent effects can also be observed at uncharged interfaces in other solvent-IL mixtures. Here, we study the microscopic structures near uncharged interfaces using Molecular Dynamics simulations varying the water concentrations in dialkylimidazolium based ILs. A comparison between the different cation and anion species highlights a crucial relation among molecular size, shape, and the preferential binding of water to the ions. The presence of water affects the local ordering of the cation species near the interface. Vibrational sum-frequency generation (SFG) experiments are performed to study the molecular structure at the air/IL interface and can verify the results from our simulations. [1] M. Jitvisate, J. R. T. Seddon, J. Phys. Chem. C 121, 18593 (2017), [2] T. Kobayashi, et al., Phys. Chem. Chem. Phys. 19, 18924 (2017)

CPP 32.10 Wed 12:00 H13

Room-temperature ionic liquids at metallic interfaces–A study of polarisation effects — •Samuel Ntim and Marialore Sulpizi — Johannes Gutenberg Universität, Mainz, Germany

Room-temperature ionic liquids (RTILs) are salts, liquid at room temperature because of their low melting points. They have peculiar properties in confined geometries and studies of such properties have become essential for many fields like energy storage, catalysis and tribology.

Due to the high electrostatic coupling between ions in the absence of a solvent, some of these peculiarities, particularly in the case of metallic confinement of RTILs, have been thought to be effects of polarisation from the confining metal.

Using classical atomistic molecular dynamics simulations, we have examined the role of polarisation effects at the interface of [BMIM][BF4] confined in gold plates. Our results provide evidence of negligible effect of polarisation on the structural, thermodynamic and dynamical properties of the RTIL.

CPP 32.11 Wed 12:15 H13

Lithium Ion Transport in Concentrated and Functionalized Ionic Liquids – A Molecular Dynamics Study — Michael Hardt[1], Andreas Heuer[1,2], and •Diddo Diddens[2] — [1]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster — [2]Helmholtz-Institut Münster (IEK-12), Ionics in Energy Storage, Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster

Ionic liquids (ILs) are promising electrolyte materials for batteries or supercapacitors. However, with the advent of high-voltage lithium ion cells, the electrochemical stability of the electrolyte is of paramount importance. Experimental strategies to enhance the electrochemical stability are the use of high lithium salt concentrations – resulting in large aggregates and thus fewer isolated molecules that are more easily decomposed – and of novel functionalized anions with delocalized charges. Furthermore, these anions tend to be asymmetric to prevent crystallization at high salt concentrations, resulting in unique solvation properties. Here, we employ Molecular Dynamics simulations to investigate the local ion coordination and ion transport properties, with special emphasis on the interplay between coordination structure and dynamical ion correlations.

CPP 32.12 Wed 12:30 H13

Molecular Dynamics Simulations of Lithium Ion Transport in Block-Copolymer Electrolytes — Len Kimms[1], Andreas Heuer[1,2], and •Diddo Diddens[2] — [1]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster — [2]Helmholtz-Institut Münster (IEK-12), Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster

Solid polymer electrolytes (SPEs) consist of a salt dissolved in an amorphous polymer melt, which typically exhibit improved safety as compared to liquid electrolytes. While the archetypal SPE is based on poly(ethylene oxide) (PEO), the use of mechanically more rigid polymers becomes necessary for lithium metal batteries that are considered to be a key technology for electric vehicles. Although a mechanically rigid polymer suppresses the growth of lithium dendrites (which in turn pose safety issues), this comes at the expense of a dramatic slowdown of the segmental mobility, and consequently also of the lithium ion dynamics. As a remedy, block copolymers that combine mechanically stable domains with ionically conducting PEO domains have been employed. In this contribution, we employ Molecular Dynamics simulations to unravel the microscopic ion transport within the conductive domains of the polymer host, and compare the results to simulations of classical PEO-based SPEs [1-3].

[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, E. Paillard, A. Heuer, *J. Electrochem. Soc.*, **2017**, 164(11), E3225-E3231

CPP 32.13 Wed 12:45 H13

Local and long-range dynamics of ionic liquids: A ^{1}H and ^{19}F NMR-study — •Elisa Steinrücken, Manuel Becher, and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstr. 6, 64289, Darmstadt, Germany

Room Temperature Ionic Liquids (RTIL) are salts with a low melting point and vapour pressure. They are usually glass forming systems with complex and heterogeneous molecular dynamics. The combination of different cations and anions opens wide ranges of chemical and physical applications and their optimization. Hence, a fundamental understanding of molecular dynamics is of crucial importance. Here, imidazolium-based RTILs with a $[\mathrm{Tf2N}]^-$ anion are in the experimental focus, with a variation of the alkyl chain length at the cation to increase structural heterogeneities. Nuclear Magnetic Resonance (NMR) provides access to glassy dynamics in wide ranges of time and length scales. Due to its isotope selectivity the dynamical behaviour of different molecules/molecular groups can be separated. In a static field gradient, we measure the self-diffusion coefficient of the cation (^{1}H) and anion (^{19}F). Field-Cycling relaxometry provides frequency-dependent relaxation times $T_1(\omega)$. The structural relaxation can be identified using support from concomitant molecular dynamics simulations. The resulting rotational correlation times are in good agreement with the findings of dynamic light scattering. Comparing long-range self-diffusion with short-range structural relaxation, we analyse cation-anion couplings, in contrast to literature no decoupling due to structural changes is observed.

CPP 33: Active Matter I (joint session BP/CPP/DY)

Time: Wednesday 9:30–13:00 Location: H4

CPP 33.1 Wed 9:30 H4

Self-assembled active systems - from individuals to a collective behaviour — •Aitor Martin-Gomez, Gerhard Gompper, and Roland G. Winkler — Forschungszentrum Juelich (ICS-2), Juelich, Germany

Active matter is comprised of agents which either convert internal energy or exploit energy from the environment to generate directed motion. Its associated out-of-equilibrium character is the origin of a number of fascinating phenomena. In particular, active systems with many internal degrees of freedom like filamentous, polymer-like structures are involved in various biological processes and exhibit novel conformational and dynamical properties. Moreover, the study of collective behavior emerging from the non-linear contributions of many individuals is an ongoing, open question. In conclusion, to shed light onto the effect of such active systems, or their passive counterparts embedded in an active environment, we perform analytical calculations combined to advanced computer simulations.

CPP 33.2 Wed 9:45 H4

Light-dependent microbial motility induces pattern formation in confinement — •Alexandros Fragkopoulos[1], Johannes Frey[1], Flora-Maud Le Menn[1], Jeremy Vachier[1], Michael Wilczek[1], Marco Mazza[1,2], and Oliver Bäumchen[1] — [1]Max Planck Institute for Dynamics and Self-Organization, D-37077 Göttingen, Germany — [2]Loughborough University, Loughborough LE11 3TU, United Kingdom

A collection of active swimmers can undergo complex dynamics due to hydrodynamic and steric interactions. For sufficiently concentrated suspensions, it is possible to form large-scale concentration patterns, where the active suspension separates into regions of high and low particle concentrations. Here we present that a collection of *Chlamydomonas reinhardtii* cells, a unicellular soil-dwelling microalgae and a model organism of puller-type microswimmers, form patterns of high and low cell density regions in confinement and under specific light conditions. We find that the motility of the cells differs significantly for different light intensities and cell densities, which regulate the pattern formation in such active suspensions. In addition, we observe that the emerged pattern follows the shape of the confinement that encloses the motile cells, which indicates that the boundaries enclosing the motile cells play a crucial role for pattern formation. Finally, by performing active Brownian dynamics simulations of active particles with the observed motility characteristics, we show that we can reproduce the experimentally observed patterns.

CPP 33.3 Wed 10:00 H4

Active Matter Invasion into Capillaries — •Felix Kempf[1], Romain Mueller[2], Erwin Frey[1], Juila Yeomans[2], and Amin Doostmohammadi[2] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München - Theresienstr. 37, D-80333 München, Germany — [2]The Rudolf Peierls Centre for Theoretical Physics - Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, UK

Biological active materials such as bacterial biofilms and eukaryotic cells thrive in confined microspaces. Here, we numerically show that combining growth dynamics with their intrinsic activity active material can use confinement as a mechanical guidance to achieve distinct modes of collective invasion. We assess the dynamics of the growing interface and classify these collective modes of invasion based on the activity of the active substance. While at small and moderate activities the active material grows as a coherent unit, we find blobs of active materials collectively detaching from the cohort above an activity threshold in a process reminiscent of the intravasation in cancer cells. We further characterise the mechanical mechanisms of transition between different modes of invasion.

CPP 33.4 Wed 10:15 H4

Collective Responses of Magnetic Swimmers in a Poiseuille Flow — •Fanlong Meng[1,2], Daiki Matsunaga[2], and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Goettingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

Magnetotactic bacteria can be focused at the radial centre of a microfluidic channel under an external magnetic field, and found to form clusters if the external magnetic field is strong or the flow speed is large [1]. However, the underlying mechanism was missing. We show that the magnetic microswimmers (not only for magnetotactic bacteria, but also applicable to synthetic magnetic microswimmers) can form interesting large-scale clusters when the magnetic attractive interaction dominates thermal fluctuations. By applying analytic techniques and conducting Brownian dynamics simulation, we provide the critical conditions for clustering of magnetic microswimmers, which matches well with the experiment. Hydrodynamic interactions between the microswimmers are also incorporated as a generalisation. Understanding the physics of magnetic active matter will help advance the cause of studying matter out of equilibrium, and provides new insight for technological applications of synthetic magnetic microrobots (for drug delivery, solution stirring, etc.) with desired collective properties. References: [1] N. Waisbord, C. T. Lefèvre, L. Bocquet, C. Ybert, C. Cottin-Bizonne, Phys. Rev. Fluids, (2016) 1, 053203 [2] F. Meng, D. Matsunaga, R. Golestanian, Phys. Rev. Lett., (2018) 120, 188101

CPP 33.5 Wed 10:30 H4

Hydrodynamic simulations of flagellated bacteria in polymer solutions and polymer networks — •Andreas Zöttl and Julia M Yeomans — University of Oxford, UK

Many cells in the human body have to move through dense complex fluids such as various cells in the extracellular matrix or bacteria in mucus. While the motion of swimming bacteria in simple Newtonian fluids can be well quantified using continuum low Reynolds number hydrodynamics, the presence of supramolecular elements such as biopolymers leads to a much more complex behavior. Although the presence of polymers generally lowers particle mobility, surprisingly, several experiments have shown that bacterial speeds increase in polymeric fluids, but there is no clear understanding why.

We perform extensive coarse-grained MPCD simulations of a bacterium swimming in explicitly modeled solutions of supramolecular model polymers of different lengths, stiffness and densities. We observe an increase of up to 60% in swimming speed with polymer density and show that this is a consequence of a non-uniform distribution of polymers in the vicinity of the bacterium leading to an effective slip. However, this alone cannot explain the large speed-up, but coupling to the chirality of the bacterial flagellum is essential. Finally we present results for swimming in crosslinked polymer networks where hydrodynamics is screened and speed enhancement is also observed.

CPP 33.6 Wed 10:45 H4

Memory-induced persistent motion — •Bernhard Georg Mitterwallner, Laura Lavacchi, and Roland Netz — Institut für theoretisch Physik, Frei Universität Berlin, Berlin, Germany

We investigate the mean-square displacement (MSD) for random motion governed by the generalized Langevin equation for different two-scale memory-kernel models: In the first model, the memory kernel consists of a delta peak and a single exponential and in the second model of the sum of two exponentials. In particular, we investigate the scenario where the long-time exponential kernel contribution is negative. The competition between positive and negative friction contributions produces an enhanced transient ballistic regime in the MSD, which is relevant for biological motility and active matter systems.

15 minutes break.

Invited Talk CPP 33.7 Wed 11:15 H4

Non-equilibrium dynamics in biological matter — •Christoph F Schmidt — Georg-August-Universität, Fakultät für Physik, Drittes Physikalisches Institut - Biophysik, Friedrich-Hund-Platz 1, 37077 Göttingen — Duke University, Department of Physics, 2316 French Family Science Center, 124 Science Drive, Durham, NC 27708, USA

Thermodynamic non-equilibrium is a defining feature of living systems on all levels of organization. Cells and tissues are built of active matter, dynamic materials with built-in force generators. Such materials self-organize in biological systems into well-ordered dynamic steady states, sustained by the dissipation of metabolic energy. The materials show striking collective phenomena on a mesoscopic scale. We used light microscopy to characterize the complex mechanical properties of and the motion and stress patterns in biological active matter, in particular the actin cortex, both in reconstituted model systems and in cells. I will introduce a method to detect and quantitate thermodynamic non-equilibrium in the dynamics of primary cilia of kidney epithelial cells using the principle of detailed balance.

CPP 33.8 Wed 11:45 H4

Enhanced rotational diffusion of squirmers in viscoelastic fluids — •Kai Qi[1], Elmar Westphal[2], Gerhard Gompper[1], and Roland Winkler[1] — [1]Theoretical Soft Matter and Biophysics, Institute for Advanced Simulation and Institute of Complex Systems, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Peter Grünberg Institute and Jülich Centre for Neutron Science, Forschungszentrum Jülich, D-52425 Jülich, Germany

Squirmers are generic models for biological microswimmers and synthetic self-propelled particles. Fluid-mediated interactions are essential for their swimming behavior, which can be strongly affected by the fluid viscoelasticity. Here, we perform mesoscale hydrodynamic simulations via the multiparticle collision dynamics (MPC) method for a spherical squirmer in a viscoelastic fluid, which is composed of MPC fluid particles and polymers. Polymers are either of phantom nature or self-avoiding. The concentration of monomers on the squirmer surface is enhanced by introducing a short-range attraction between the squirmer and polymers. This leads to a decrease of the rotational diffusion for a passive colloid in the presence of polymers. Self-propulsion reduces the monomer concentration on the surface and the squirmer's rotational diffusion is enhanced considerably, up to a factor 20 for phantom polymers. The actual change of the rotational diffusion D_r depends on the polymer length. An increasing polymer length reduces D_r^0 of the passive colloid, but D_r of the squirmer is enhanced. Both effects contribute to the obtained substantial increase of the ratio D_r/D_r^0.

CPP 33.9 Wed 12:00 H4

Modelling coordinated motion in simplest multicellular animals — •Stephan Meschede[1] and Pawel Romanczuk[2] — [1]Department of Physics, Humboldt Universität zu Berlin — [2]Institute for Theoretical Biology, Department of Biology, Humboldt Universität zu Berlin

Placozoa, Trichoplax adhaerens, are structurally simplest known multicellular animals. Their bodies are flat and irregular, up to few milimeters in diameter and $10-15\mu m$ thick [1]. They consists of three layers, an upper and a lower epithelium enclosing a fiber cell layer. The Trichoplax body plan is completely decentralized without any hierarchical structure or a central nervous system. However, they are capable of amoeba-like, coordinated active motion on substrates through ciliary locomotion. We show that individual Trichoplax motion behavior can be modeled as a two-dimensional 'sheet' of active particles coupled through elastic forces, building upon previous models of cellular migration model proposed by Szabo et al [2]. We discuss the emergence of coordinated motion and the role of animal size and elastic coupling strength for the stochastic motility. Our aim is to understand how the self-organized active sheet dynamics shapes and constrains the motion behavior of these simple animals and their ability to navigate the environment.

[1]: Miller, D. J., & Ball, E. E. (2005). Animal Evolution: The Enigmatic Phylum Placozoa Revisited. Current Biology, 15(1), 26-28.

[2]: Szabó, B. et al.(2006). Phase transition in the collective migration of tissue cells: Experiment and model. Phys. Rev. E, 74(6), 1-5.

CPP 33.10 Wed 12:15 H4

Phase space geometry of reaction–diffusion systems — •Fridtjof Brauns, Jacob Halatek, and Erwin Frey — Arnold Sommerfeld Center for Theoret- ical Physics, Ludwig-Maximilians-Universität München, Germany

Self-organized pattern formation — typically studied in terms of spatially extended dynamical systems — is as ubiquitous in nature as it is difficult to deal with conceptually and mathematically. We build on the phase space geometric methods of Nonlinear Dynamics, using geometric structures like nullclines and fixed points, to develop a comprehensive theory for two-component mass-conserving reaction–diffusion systems — a paradigmatic model class for pattern formation, e.g. intracellular polarization. A dissection of space into (notional) compartments enables us to characterize the spatio-temporal dynamics based on the ODE phase space of local reactions. Diffusive coupling leads to mass redistribution between the compartments which, in turn, changes the local phase space properties.

We show that all aspects of pattern formation, from linear instability and excitability to the bifurcations of stationary patterns, can be extracted from the geometric features of the line of chemical equilibria in phase space. Furthermore, our analysis points towards a deep connection between the far from equilibrium reaction–diffusion dynamics to phase separation of binary mixtures near equilibrium, and thus offers a new perspective on phase separation far from equilibrium.

CPP 33.11 Wed 12:30 H4

Diffusive dynamics of complex particles in active colloidal suspensions of motile algae — •Florian von Rüling and Alexey Eremin — Institute of Physics, Otto von Guericke Universität Magdeburg, Germany

We report experimental studies on the dynamics of complex passive particles in the presence of motile algae Chlamydomonas reinhardtii in thin capillaries. Employing video microscopy and particle tracking algorithm, the enhancement of the diffusion of elongated particles due to interactions with the microswimmers was explored. Depending on the number of motile algae, the translational and rotational diffusion constants of doublets of silica beads close to a solid boundary can be increased by several orders of magnitude in comparison to purely Brownian motion. At a high concentration of Chlamydomonas reinhardtii, the algae formed dense dynamic clusters at the lower capillary wall. In this state of the system, swimming and clustering algae interact with passive particles. Clustering algae can restrict both translational and rotational dynamics of the silica doublets. We explore the effect of the motion of algae in such active clusters on the dynamic of the passive silica doublets.

CPP 33.12 Wed 12:45 H4

Self-propelled Dipolar Nanocubes — •Martin Kaiser[1], Sofia Kantorovich[1,2], Yeimy Martinez[3], and Annette Schmidt[3] — [1]University of Vienna, Austria — [2]Ural federal University, Russia — [3]Universität zu Köln, Germany

Microscopic active particles, including self-propelled cells, microorganisms and artificial swimming colloids, have gained a lot of attention due to their relevance in such important fields as biology, biomedicine, nanoscience and nanotechnology. The term "active" describes the ability of certain particles or units, to convert energy from their environment into motion, hence, kinetic energy.

In this study, we use active matter to create a new type of nanomotor, which is oriented by an applied magnetic field and propelled by an active particle. One of those units consists of a dipolar cube that can be directed due to its interaction with a magnetic field. A non-dipolar active particle attached to the cube, with a propulsion force directed into the cubes centre of mass, creates a field controlled swimming unit.

This scenario is investigated using molecular-dynamic simulations, setting the above described unit in an obstacle free environment while applying a constant magnetic field.

In collaboration with Dr. Schmidt from the University of Cologne, those nanomotors are also investigated experimentally.

CPP 34: Two-dimensional Materials III (joint session HL/CPP)

Time: Wednesday 9:30–13:00 Location: H36

CPP 34.1 Wed 9:30 H36

Defect dominated charge transport and fermi level pinning in TMDC/metal contacts — •Kai Sotthewes, Rik van Bremen, Edwin Dollekamp, Harold Zandvliet, and Pantelis Bampoulis — Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, P.O. Box 217, 7500AE Enschede, The Netherlands

Understanding the electron transport through transition metal dichalcogenides (TMDCs) based semiconductor/metal junctions is vital for the realization of future TMDC based (opto-) electronic devices. Strong Fermi level pinning was observed in TMDC based devices, reducing the tenability of the Schottky barrier height. We use conductive atomic force microscopy to construct nanoscopic metal-TMDC junctions in order to understand the Fermi level pinning mechanism on TMDCs and the influence of defects on the electron transport. The barrier heights of the pristine surface can be explained by metal induced gap states (MIGS), inducing partial Fermi level pinning. The Schottky barrier height further reduces (Fermi level pinning increases) at defects, where the magnitude of the decrease depends on the metal contact. These defects provide low-resistance conduction paths in TMDC-based nanodevices and will play a prominent role as the device junction contact area decreases in size.

CPP 34.2 Wed 9:45 H36

Localized quantum emitters in Van der Waals crystals — •Amlan Mukherjee[1], Nathan Chejanovsky[1,2], Youngwook Kim[2], Durga Dasari[1,2], Jurgen H. Smet[2], and Jörg Wrachtrup[1,2] — [1]3rd Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Point defects in semi-conductors are renowned for single photon emission apart from having important implications on optical and transport properties of their host crystal. Various two dimensional Van der Waals (2D) crystals can provide a plethora of defects [1][2] and have revolutionized scientific research with unique phenomena related to their reduced dimensional. We summarize optical investigations of localized quantum emitters in 2D semi-conductors with sub band-gap excitation energizes, emphasizing those in hexagonal boron nitride that exhibit para-magnetic responses to applied external magnetic fields.

References: [1] Chejanovsky, N. et al. Nano letters 2016, 16, 7037-7045. [2] Chejanovsky, N. et al. Scientific reports 2017, 7, 14758 (1-14).

CPP 34.3 Wed 10:00 H36

High magnetic field measurements of interlayer excitons in van der Waals heterostructures — •Johannes Holler[1], Michael Kempf[1], Jonas Zipfel[1], Mariana Ballottin[2], Anatolie Mitioglu[2], Philipp Nagler[1], Fabian Mooshammer[1], Alexey Chernikov[1], Peter Christianen[2], Christian Schüller[1], and Tobias Korn[3] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]High Field Magnet Laboratory (HFML EMFL), Radboud University Nijmegen, Netherlands — [3]Institut für Physik, Universität Rostock, Germany

In the recent years, research in the field of two-dimensional materials has intensified a lot. Besides graphene, the most prominent representatives for this field are the transition metal dichalchogenides. These materials exhibit interesting physics in the monolayer, such as spin-valley locking, and by combining them to heterostructures new excitonic properties emerge.

Here, we study $MoSe_2$-WSe_2 heterostructures, which create a type-II band alignment. This results in a spatial separation of the electron-hole pairs, leading to the formation of interlayer excitons (IEXs). In low-temperature photoluminescence measurements in magnetic fields up to 30T, we observe a giant valley-selective splitting and a resulting near-unity valley polarization. Furthermore, we probe the valley dynamics of the IEX in dependence of the magnetic field, detecting very long lifetimes in contrast to intralayer excitons. We are able to observe the build-up of the valley polarization after unpolarized excitation, revealing different dynamics and lifetimes for the different valleys.

CPP 34.4 Wed 10:15 H36

Tunable 2D superlattices in graphene — •Robin Huber[1], Martin Drienovsky[1], Andreas Sandner[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institue of Experimental and Applied Physics, University of Regensburg, Germany — [2]National Institute for Materials Science, Tsukuba, Japan

One fascinating way to study the effect of superlattices on graphene are graphene/hBN heterostructures in which moiré superlattices with lattice periods of about 10 nm can be created. These systems made it possible to observe e.g. the famous Hofstadter butterfly in all its beauty. Here we present an alternative method to induce tunable superlattice effects in graphene by the combined action of a global silicon backgate and a patterned bottom gate made from few layer graphene using standard e-beam lithography techniques. We show low temperature transport measurements on an artificially fabricated and gate tunable 2D superlattice in graphene with a lattice period of 40 nm. By switching on a 2D periodic charge carrier density modulation additional Dirac peaks can be observed which are the source of additional Landau fans in magnetotransport. Due to the interplay between the lateral 2D superlattice and a magnetic field, features of the Hofstadter butterfly energy spectrum can be resolved. In addition we show magnetotransport data at an elevated temperature of 120 K where Landau quantization vanishes but Brown-Zak oscillations, which are caused by the 2D periodic potential, are still visible.

CPP 34.5 Wed 10:30 H36

Charge carrier localization in molybdenum disulfide nanobubbles due to the interplay of surface wrinkling, strain, and dielectric confinement — •Christian Carmesin, Michael Lorke, Matthias Florian, Daniel Erben, Tim O. Wehling, and Frank Jahnke — Institut für Theoretische Physik, Universität Bremen

The observation of quantum light emission from atomically thin transition metal dichalcogenides has opened a new field of applications for these material systems. The corresponding charge carrier localization has been linked to defects and strain, however open questions remain about the microscopic origin. We demonstrate that bending of two-dimensional layers leads to surface wrinkling due to bond deformation within the atomically thin sheet. The resulting strain-field facilitates strong charge carrier localization due to its pronounced influence on the band gap. Additionally, we consider confinement as a result of local changes of the dielectric environment and show that both effects contribute to modified electronic states and optical properties. The interplay of surface wrinkling, strain-induced confinement and local changes of the dielectric environment is demonstrated for the example of nanobubbles that form when monolayers are deposited either on substrates or other two-dimensional materials.

CPP 34.6 Wed 10:45 H36

Electric field control of interlayer excitons in MoS2/WS2 heterobilayers — •Fabian Kronowetter[1], Jonas Kiemle[1], Florian Sigger[1,2], Alexander Holleitner[1,2], and Ursula Wurstbauer[1,2,3] — [1]Walter Schottky Institut and Physics-Department, Technical University of Munich, Germany — [2]Nanosystems Initiative Munich (NIM), Germany — [3]Institute of Physics, WWU Münster, Germany

Ensembles of interlayer excitons (IXs) are intriguing systems to explore classical and quantum phases of interacting bosonic ensembles with enlarged lifetimes due to reduced overlap of the electron-hole wave functions. We demonstrate electric field control of the IX in MoS2/WS2 heterobilayer embedded in a field effect structure with few layer hexagonal boron nitrite (hBN) as insulator and few-layer graphene as gate-electrodes. We observe a multiplet structure in the IX emission band even at room temperature. Stark shift measurements reveal the presence of a finite out-of plane dipole of the IX. The different strength of the dipole and a distinct temperature dependence identify the IXs to stem from optical interband transitions with electrons and holes located in different valleys of the heterostructures. For the lowest emission line, we observe field dependent level anti-crossing at low temperatures. We discuss this behavior in terms of coupling of electronic states from the two TMDC monolayers. Our results demonstrate the design of novel nano-quantum materials prepared from artificial van der Waals solids with the possibility to in-situ control their physical properties via external stimuli such as electric fields.

15 min. break

CPP 34.7 Wed 11:15 H36

excitons localized by physisorbed gas molecules in MoSe2 monolayer — •Tommaso Venanzi[1,2], Stephan Winnerl[1], Alexej Pashkin[1], Manfred Helm[1,2], and Harald Schneider[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany

In the study of 2D materials an extremely relevant topic is the presence of defects. We have studied excitons localized by physisorbed gas molecules in MoSe2 monolayer by means of low-temperature photoluminescence. We have investigated how the localized exciton depends on temperature taking care of the effects of laser irradiation. We observe a red-shift of the photoluminescence peak with temperature that is not only addressable to renormalization of the bandgap or thermal instability of the localization. On the other hand we observe a blueshift of the peak when increasing the laser irradiation dose. Finally we propose a physical mechanism that can explain our experimental observations.

CPP 34.8 Wed 11:30 H36

Silicene passivation by few-layer graphene — •Jakob Genser[1], Viktoria Ritter[1], Daniele Nazzari[1], Ole Bethge[2], Emmerich Bertagnolli[1], and Alois Lugstein[1] — [1]Institute of Solid State Electronics, Technische Universität Wien, Gußhausstraße 25-25a, 1040 Vienna, Austria — [2]Infineon Technologies Austria AG, Siemensstraße 2, 9500 Villach, Austria

Silicene is of foremost interest for the development of next generation, high performance devices, due to its ultra-high carrier mobility combined with a tuneable bandgap and good integrateability into the current silicon based semiconductor industry. However, the synthesis of silicene remains challenging and thus far is only achieved under UHV conditions, whereas exposure to air leads to an immediate degradation. Therefore, the stabilization of silicene at ambient conditions is essential for its characterization, future processing and device integration. Here, we demonstrate the first in-situ encapsulation of 4x4 silicene grown on Ag(111) by exfoliated few-layer graphene (FLG) flakes. This encapsulation method allowed subsequent highly detailed Raman analysis that so far has only been possible by means of in-situ Raman measurements. The acquired data proved that FLG capping serves as an effective passivation layer, preventing degradation of silicene for up to several days. Additional polarization-dependent measurements showed that the symmetry properties of silicene remain unaltered by the capping process. Furthermore, the experiments demonstrated the compatibility between graphene and silicene, representing a step forward towards the possible integration of silicene into 2D heterostructures.

CPP 34.9 Wed 11:45 H36

Internal structure and ultrafast dynamics of interlayer excitons in van der Waals heterostructures — •Philipp Merkl[1], Philipp Steinleitner[1], Fabian Mooshammer[1], Kai-Qiang Lin[1], Philipp Nagler[1], Johannes Holler[1], Christian Schüller[1], John M. Lupton[1], Tobias Korn[1], Simon Ovesen[2], Samuel Brem[2], Ermin Malic[2] und Rupert Huber[1] — [1]Department of Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]Department of Physics, Chalmers University of Technology, SE-41258 Göteborg, Sweden

In heterostructures of transition metal dichalcogenides, electrons and holes residing in adjacent monolayers can bind into spatially indirect excitons. Even though these interlayer bound pairs have attracted tremendous interest owing to their strong promise for novel optoelectronics and valleytronics, their binding energies have not been directly measured. Here we introduce a direct ultrafast access to Coulomb correlations acting between monolayers. For the prototypical case of WSe2/WS2 hetero-bilayers, phase-locked mid-infrared pulses allow us to measure the binding energy of interlayer excitons of 118 meV by revealing a novel 1s-2p resonance, well explained by a fully quantum mechanical model. Furthermore, we trace how an exciton gas photogenerated in the WSe2 layer directly transforms into interlayer excitons, without a strong intermediate phase of unbound electron-hole pairs. Depending on the stacking angle, intra- and interlayer species coexist on picosecond scales and relax into quantum confined states in moiré-induced nanodots.

CPP 34.10 Wed 12:00 H36

Plasmonic Coupling and Engineering of Single Photon Emitters in WSe2 Monolayers — •Oliver Iff[1], Nils Lundt[1], Simon Betzold[1], Łukasz Dusanowski[1], Magdalena Moczała-Dusanowska[1], Laxmi Narayan Tripathi[1], Young Jin Lee[2], Soon-Hong Kwon[2], Sven Hoefling[1,3], and Christian Schneider[1] — [1]Technische Physik, Universität Würzburg, Wuerzburg, Germany — [2]Department of Physics, Chung-Ang University, Seoul, South Korea — [3]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, UK

Single photon sources are an important building block in quantum technologies. The rediscovery of transition metal dichalcogenides this century revealed the availability of quantum emitters in monolayers of WSe2 or MoSe2. Here, we investigate the resonant coupling of such emitters to metallic nanostructures of different shapes and sizes. Auto correlation measurements prove their single photon emission as well as lifetime measurements unveil a reduction in their decay times, confirming the coupling between the metal surface and the quantum emitters. Furthermore, by utilizing an array of gold nanopillars as well as strain-engineering and -tuning of monolayers, site-controlled positioning of localized emitters is possible and represents an important step towards their reproducible manipulation. These findings demonstrate the potential of transition metal dichalcogenide based, strain engineered devices for quantum electrodynamic systems.

CPP 34.11 Wed 12:15 H36

Understanding the formation of interlayer excitons in the case of MoS_2 on GaSe. — •Christian Wagner[1,2], Mahfujur Rahaman[2], Dietrich R.T. Zahn[2], and Sibylle Gemming[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany

The fabrication of hybrid van-der-Waals heterostructures of two-dimensional nano materials is an emerging field of study: The (weak) electronic interaction between two layers is often reasonably described by a perturbation of the physical effects of the isolated layers, such as electrostatic doping and screening of intralayer excitons. However, it turns out that this picture of the weak interaction is not exhaustive in terms of optical properties: the formation of bound excitons from electrons of one layer and the holes from another layer yields the formation of interlayer excitons. These states are measured experimentally by photoluminescence and photocurrents, e.g. in the case of MoS_2 on GaSe due to type-II band alignment.

This contribution elucidates the conditions for the formation of interlayer excitons from a first-principles point of view. For this, first-principles studies of a minimal test system are conducted. One perspective is then to predict these states as a function of the heterostack in order to specifically taylor efficient solar cells.

CPP 34.12 Wed 12:30 H36

Transfer of electrodeposited MoS_2 to silicon substrate for electronic devices — •Talha Nisar, Torsten Balster, and Veit Wagner — Jacobs University Bremen gGmbH, Campus Ring 1, 28759, Bremen, Germany

Molybdenum disulfide is a promising candidate for future electronics due to its 2 dimensional nature. It can be deposited by various methods such as mechanical exfoliation and chemical vapor deposition (CVD). In our approach we use electrodeposition as an alternative large area deposition method to CVD. For this purpose a MoS_4 ion precursor is used in the anodic regime. The electrodeposited layer consists of MoS_3 as confirmed by Raman and XPS measurements. Such layers are converted to MoS_2 by post annealing at temperature above 450°C. Raman analysis shows that the crystallinity of such film improves with higher post annealing temperatures. In addition, UV-Vis and AFM measurements confirm MoS_2 formation in flakes with smooth surface. We demonstrated that these layers can successfully be mechanically transferred to a SiO_2/Si.

CPP 34.13 Wed 12:45 H36

Optical properties of Monolayer MoS_2 exposed to helium ions — Julian Klein[1,2], •Sergio Rey Puentes[1], Michael Lorke[3], Matthias Florian[3], Florian Sigger[1,2], John Cerne[4], Jakob Wierzbowski[1,2], Kai Müller[1,2], Lukas Sigl[1,2], Takashi Taniguchi[5], Kenji Watanabe[5], Michael Kaniber[1,2], Ursula Wurstbauer[1,2], Michael Knap[6], Richard Schmidt[6], Jonathan Finley[1,2], and Alexander Holleitner[1,2] — [1]Walter Schottky Institut and Physik Department, Technische Universität München, Garching, Germany — [2]Nanosystems Initiative Munich (NIM), Munich, Germany — [3]Institut für Theoretische Physik, Universität Bremen, Bremen, Germany — [4]Department of Physics, University at Buffalo, The State University of New York, Buffalo, USA — [5]National Institute for Materials Science, Tsukuba, Japan — [6]Department of Physics and Institute for Advanced Study, Technical University of Munich, Garching, Germany

We present a spectroscopic study on mono- and few-layers of 2H stacked MoS_2 and WSe_2 exposed with helium ions. Distinct changes of the first-order Raman bands, additional defect luminescence and strong modification of the intrinsic valley spin relaxation properties are observed. The exposed locations were investigated by Raman spectroscopy, low-temperature confocal micro-photoluminescence (μ-PL) and atomic force microscopy (AFM). Our results demonstrate the potential of helium ion microscopy applied to 2D layered materials for modifying intrinsic optical properties and fundamental understanding of disorder.

CPP 35: Plasmonics III (joint session O/CPP)

Time: Wednesday 10:30–13:15 Location: H8

CPP 35.1 Wed 10:30 H8

Plasmon-assisted resonant electron tunneling in a scanning tunneling microscope junction — Shuyi Liu[1], Martin Wolf[1], and •Takashi Kumagai[1,2] — [1]Fritz-Haber Institute of the Max-Planck Society — [2]JST-PRESTO

Plasmon-induced phenomena have attracted increasing attention due to diverse applications in nanoscale science and technology [1]. Plasmonic nanocavities play a particularly important role because of their ability to confine light to nanometric volumes and generate a strong field enhancement. We report plasmon-assisted resonant electron tunneling from an Ag or Au tip to field emission resonances (FERs) of a Ag(111) surface induced by CW laser excitation of a scanning tunneling microscope (STM) junction at visible wavelengths [2]. As a hallmark of the plasmon-assisted resonant tunneling, we observe a downshift of the first peak in the FER spectra by a fixed amount equal to the incident photon energy. STM-induced luminescence measurement for the Ag and Au tip reveals the clear correlation between the laser-induced change in the FER spectra and the plasmonic properties of the junction. Our results clarify a novel resonant electron transfer mechanism in a plasmonic nanocavity. References: [1] M. L. Brongersma, N. J. Halas, P. Nordlander, Plasmon-induced hot carrier science and technology. Nat. Nanotechnol. 10, 25-34 (2015). [2] S. Liu, M. Wolf, T. Kumagai, Phys. Rev. Lett. in print, 10.1103/PhysRevLett.121.226802.

CPP 35.2 Wed 10:45 H8

Investigation of plasmon assisted light emission from heteroepitaxial system of Co islands on Cu(111) by scanning tunneling microscopy — •Vibhuti Rai[1], Kevin Edelmann[1,2], Lars Wilmes[1], Lukas Gerhard[1], and Wulf Wulfhekel[1,2] — [1]Institut für Nanotechnologie, Karlsruher Institut für Technologie, 76344 Eggenstein-Leopoldshafen, Germany — [2]Physikalisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

Scanning tunneling microscopy (STM) with optical access allows systematic and controlled investigation of light emission from nanometersized structures[1]. Here, plasmon mediated light emission from a heteroepitaxial system of bilayer and trilayer Co islands on Cu(111) is studied in ultra-high vacuum at low temperature (4.4 K). Electrical spectroscopy and optical spectroscopy were performed on an image size of 40 x 40 nm where an optical spectrum was taken at every point of a 160 x 160 grid. These measurements show the effect of geometric cavity alteration and the associated resonance shift, influence of dielectric constant of the sample and the tip, and modulation of emission intensity by Friedel oscillation. Interestingly, the results indicate that the difference in the yield of inelastic tunneling dominates over the difference of the gap plasmon resonance.

[1] K. Edelmann et al. Rev. Sci. Instrum. accepted for publication.

CPP 35.3 Wed 11:00 H8

Photon super-bunching from a metal-metal tunnel junction — Christopher C. Leon[1], Anna Rosławska[1], •Abhishek Grewal[1], Olle Gunnarsson[1], Klaus Kuhnke[1], and Klaus Kern[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Institut de Physique, École Polytechnique Fédérale de Lausanne, Switzerland

Generating correlated photon pairs at the nanoscale is a prerequisite to creating highly-integrated optoelectronic circuits that perform quantum computing tasks based on heralded single-photons. Here, we report on the observation of bunched light emission from a generic tunnel junction under DC-bias. Using LT-STM coupled with Hanbury Brown-Twiss interferometer we probe the dynamics of the photon stream emitted by a metal-metal junction. The inelastic tunneling events of single electrons produce a plasmonic emission whose bunching factor can be 17 (super-bunching) when measured with 53 picosecond instrument resolution. Spectral filtering indicates that two photons of energy higher and lower than half the tunneling electron energy participate in bunching.

We show that mechanisms such as mechanical instabilities at the tip apex, electron co-tunneling, and electronic detection artifacts can be excluded, confirming the non-triviality of the emission. The $1e^- \rightarrow n\gamma$ process is promoted by the localized Purcell effect in conjunction with optical nonlinearities due to inversion symmetry breaking at the tunnel junction. The results suggest that an optoelectronic component useful for quantum computing can be miniaturized to the atomic scale.

CPP 35.4 Wed 11:15 H8

Simulating ultrashort light pulses in STM tunnel junctions — •Alexander Neef[1], Dominik Peller[2], Rupert Huber[2], and Jascha Repp[2] — [1]Fritz-Haber-Institute of the MPG, D-14195, Berlin,Germany — [2]Fakultaet fuer Physik, Universitaet Regensburg, D-93040 Regensburg, Germany

Combining ultrafast lightwave control and scanning tunneling miscroscopy (STM) recently opened the door to atomic-scale femtosecond imaging [1,2]. In lightwave STM, a THz field transient is coupled into the tunneling junction to apply an ultrashort bias voltage. The near-field waveform at the tip apex controls single-electron tunneling with combined femtosecond temporal and sub-Å spatial precision. Exploiting this process, single-molecule THz vibrations could be resolved directly in space and time [2]. The mechanism of sub-cycle tunneling control crucially depends on the exact shape of the near-field waveform in the junction, which is determined by interactions of the incoupled terahertz pulses with tip and substrate. To understand the effect of these near-field interactions on the voltage pulses in the junction, we carried out finite element simulations in the frequency domain. The resulting near-field waveforms coincide with experimental results. To further optimize the near-field transients, we study different geometries of the junction.

[1] T. L. Cocker et al., Nature Photon. 7, 620-625 (2013)
[2] T. L. Cocker, D. Peller, P. Yu, J. Repp, and R. Huber, Nature 539, 263 (2016).

CPP 35.5 Wed 11:30 H8

Advances with Attosecond Electron Pulse Trains in Ultrafast Transmission Electron Microscopy — •Thomas Rittmann[1], Katharina E. Priebe[1], Christopher Rathje[1,2], Sascha Schäfer[1,2], Sergey V. Yalunin[1], Thorsten Hohage[3], Armin Feist[1], and Claus Ropers[1] — [1]4th Physical Institute - Solids and Nanostructures, University of Göttingen, Germany — [2]Institut für Physik, University of Oldenburg, Germany — [3]Institut für Numerische und Angewandte Mathematik, University of Göttingen

In an ultrafast transmission electron microscope (UTEM), inelastic scattering between a free-electron beam and strong optical near fields [1] allows for a coherent manipulation of the electron quantum state. In this mechanism, the optical field imprints a sinusoidal phase modulation on the electron wave function, which, after subsequent dispersive propagation, results in a temporal electron density modulation [2].

Here, we employ a second electron-light interaction at varied propagation distances with accurately controlled phase delay, and reconstruct the temporal shape of the electron density at each distance with our quantum state tomography algorithm 'SQUIRRELS' [3]. We demonstrate the compression of electron pulses into trains of attosecond bursts and explore the improvement of pulse durations by minimizing phase averaging effects. Such pulse trains will promote new forms of ultrafast electron microscopy with attosecond resolution.

[1] B. Barwick *et al.*, Nature **462**, 902-906 (2009)
[2] A. Feist *et al.*, Nature Physics **12**, 1000-1004 (2016)
[3] K. Priebe *et al.*, Nature Photonics **11**, 793-797 (2017)

CPP 35.6 Wed 11:45 H8

A versatile setup utilizing shaped optical pulses and time-resolved photoemission electron microscopy to disentangle the ultrafast local response of nanostructured surface systems — •Sebastian Pres[1], Bernhard Huber[1], Daniel Fersch[1], Enno Krauss[2], Daniel Friedrich[2], Victor Lisinetskii[1], Matthias Hensen[1], Bert Hecht[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Nano-Optics & Biophotonics Group, Experimentelle Physik 5, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The possibility to disentangle local field dynamics on nanometer length scales is an important prerequisite for the exploration of interactions between nanostructures and nearby quantum systems.

We combine time-resolved aberration-corrected photoemission electron microscopy, enabling sub-10 nm spatial resolution, with a widely tunable laser source generating sub-20 fs excitation pulses at 1 MHz repetition rate. Phase-stable pulse sequences are formed by liquid-crystal-based pulse shaping and characterised by Fourier-transform spectral interferometry. A detailed knowledge of each pulse sequence's amplitude and phase structure during the measurement allows to quantitatively analyse the influence of the pulse shape and laser spectrum on resulting time-resolved multidimensional spectroscopy signals. Using coherent 2D nanoscopy [1] we investigate local field dynamics within a plasmonic nanoslit resonator.

[1] M. Aeschlimann et al., *Nat. Photonics*, Vol. 9 (2015)

CPP 35.7 Wed 12:00 H8

Dynamic imaging of plasmonic nanostructures with an ultrafast point-projection electron microscope — •Germann Hergert[1], Andreas Wöste[1], Jan Vogelsang[1], Dong Wang[2], Petra Gross[1], and Christoph Lienau[1] — [1]Institut für Physik, Carl von Ossietzky Universität, 26129 Oldenburg, Germany — [2]Institut für Werkstofftechnik, TU Ilmenau, 98693, Germany

The motion of electrons inside metallic nanostructures defines their optical properties. The study of this electron motion requires microscopes with few-fs time and nm-spatial resolution. Ultrafast electron microscopy (UEM) is a promising approach towards this goal, combining the spatial resolution of electron microscopes with the temporal resolution of ultrashort laser pulses. So far, the mesoscopic distance between sample and electron emitter limits the temporal resolution in UEM to 100fs.

We solve this problem with a novel electron source in form of a conical gold taper, without direct illumination of the apex. Light is coupled to surface plasmons on the shaft of the tip, which propagate towards the apex, where they cause electron emission.

Implementing this source in our ultrafast point-projection microscope allows minimal sample-emitter distances and therefore enhanced temporal resolution of 20fs [1]. We use this microscope to observe the ultrafast expansion of a photoemitted electron cloud inside a plasmonic nanoresonator in real space, and in addition, we observe a streaking of the probing electrons by the photoemitted charges.

[1] J. Vogelsang et al., Light: Science & Applications 7, 55 (2018)

CPP 35.8 Wed 12:15 H8

Quantum Pathway Interference between Surface Plasmon Polariton and Photon — •David Janoschka, Pascal Dreher, Michael Horn- von Hoegen, and Frank J. Meyer zu Heringdorf — Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany

It is well known that the coherent superposition of light and surface plasmon polaritons (SPPs) at a surface leads to an interferometric mixture of both their electromagnetic fields. At metal surfaces, electrons can be liberated from this mixture by a nonlinear electron emission pathway. In pump probe experiments, the time dependence of the fields has been used to image the propagation of SPPs in a photoemission electron microscope (PEEM). Strictly speaking, the contrast in the microscope arises from the absorption of either photons, SPPs, or both. Here we use Fourier techniques to disentangle the different contributions of photons and SPPs to the electron emission. In addition to the individual contributions of photons and SPPs we find emission pathways that can only be explained by a quantum interference of SPP and photon.

CPP 35.9 Wed 12:30 H8

Revealing local mode dynamics within a plasmonic nanoslit cavity by time-resolved photoemission electron microscopy — Bernhard Huber[1], Daniel Friedrich[2], Enno Krauss[2], Sebastian Pres[1], Philipp Grimm[2], Daniel Fersch[1], Julian Lüttig[1], Victor Lisinetskii[1], •Matthias Hensen[1], Bert Hecht[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Am Hubland, 97074 Würzburg, Germany

Plasmonic cavities are known for supporting discrete modes upon resonant excitation with light. The associated characteristic pattern of intense electromagnetic hot-spots can be exploited to enhance light-matter interaction and to enable strong coupling of distinct cavities over a micrometer distance [1] or to strongly couple single excitons and plasmons at room temperature [2]. Here, we disentangle the local field dynamics of individual hot-spots within a nanoslit resonator with a spatial resolution of < 10 nm by combining time-resolved photoemission electron microscopy (PEEM) and a 1 MHz NOPA system. Interestingly, we detect local differences of rather global properties such as the Q-factor and resonance frequency. By using the concept of quasinormal modes we explain these notable local differences, which will be experienced by, e.g., quantum emitters, with a non-negligible influence of adjacent resonator modes.

[1] M. Aeschlimann et al., *Light Sci. Appl.* 6, e17111 (2017)
[2] H. Groß et al., *Sci. Adv.* 4, eaar4906 (2018)

CPP 35.10 Wed 12:45 H8

Direct optical excitation of dark plasmons for hot electron generation. — •Dominik Höing[1], Niclas Müller[2], Florian Schulz[1], Stephanie Reich[2], and Holger Lange[1] — [1]Institut für Physikalische Chemie, Universität Hamburg, Sedanstraße 19, VG1-045, 20146 Hamburg — [2]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, Raum 1.2.42, 14195 Berlin

Plasmonic gold nanoparticles (AuNP) are of great interest because of their ability to generate hot charge carriers, which can play a key role in photoinduced catalysis [1]. Previous studies have shown that the generation of hot carriers depends on whether or not the photon energy is larger than the threshold for interband transitions while exciting at the plasmon resonance seems to have a low effect [2]. A possible explanation might be a significant contribution of radiative energy losses during the plasmon decay. Dark plasmon modes, which can be observed in AuNP multilayers, do not couple to the far field and might allow to reduce such losses [3]. An experimental access to the efficiency of hot carrier generation is transient absorption spectroscopy. It has proven to be a reliable method as it allows assessing the initial temperature of the electrons after excitation and thermalization [4]. In our contribution we investigate the effect of radiative losses on the excitation of hot electrons, by comparing the hot electron dynamics in AuNP mono- and bilayers.

[1] ACS Cent. Sci. 2017, 3, 482-488 ; [2] J. Phys. Chem. Lett. 2017, 8, 19, 4925-4929 ; [3] ACS Photonics 2018, 5, 10, 3962-3969 ; [4] Chem. Rev. 2011, 111, 3858-3887.

CPP 35.11 Wed 13:00 H8

Angle-resolved plasmoemission from strong SPP fields — •Pascal Dreher, David Janoschka, Michael Horn-von Hoegen, and Frank Meyer zu Heringdorf — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstrasse 1-21, 47057 Duisburg, Germany

Recent efforts to observe strong-field phenomena in photoemission from metal surfaces have utilized the local enhancement of optical near-fields in nanostructures such as nanotips. On flat metal surfaces high field intensities can be achieved by femtosecond surface plasmon polariton (SPP) pulses. Here we exploit the spatio-temporal nanofocusing of SPPs in Archimedean vortex lenses [1] to achieve particularly strong plasmonic near fields with well-known field distributions on flat Au(111) surfaces. A spectroscopic photoemission electron microscope is employed to detect the electrons which are emitted from the surface by the simultaneous absorption of up to seven SPP quanta. In angle-resolved plasmoemission spectra (ARPLES) we observe signatures which can be attributed to above-threshold plasmoemission from the Au(111) Shockley surface state into SPP-dressed free electron states. The ponderomotive energy that the emitted electrons gain within the strong plasmonic nanofocus is determined from spatially-resolved plasmoemission spectra. The ponderomotive energy provides us with a direct measure for an absolute value of the transverse electric field strength of the SPP in the focus point.

[1] Spektor G, et al., Science 355, 1187 (2017)

CPP 36: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge V (joint session O/CPP/DS/TT)

Time: Wednesday 10:30–13:15 Location: H9

Topical Talk CPP 36.1 Wed 10:30 H9

Theoretical Investigations of Electrochemical CO2 Reduction — •Karen Chan — Department of Physics, Technical University of Denmark

The electroreduction of CO_2 has the potential to store energy from intermittent renewable sources and to produce carbon-neutral fuels and chemicals; In this talk, I will discuss new developments in modeling the electrochemical interface. I will then present the application of these models of the interface to CO_2 reduction: the determination of reaction pathways and kinetics on transition metals, field and solvation effects, pH effects on C_2 product selectivity, and implications for catalyst design.

Topical Talk CPP 36.2 Wed 11:00 H9

First-principles approach to model electrochemical reactions at the solid-liquid interface — •Mira Todorova, Sudarsan Surendralal, and Jörg Neugebauer — MPI für Eisenforschung, Düsseldorf

Processes at solid-liquid interfaces are at the heart of many present day technological challenges related to the improvement of battery materials, electro-catalysis, fuel cells, corrosion and others. Describing and quantifying the underlying fundamental mechanisms is equally challenging for experimental and theoretical techniques.

Utilizing concepts from semiconductor physics, we have developed a novel potentiostat design, which enables us to perform ab initio calculations under controlled bias conditions. Easily applied in standard density functional theory codes, it controls the electrode potential of the system by tuning the excess charge of the working electrode and allows us to obtain direct insight into key mechanisms of electrocatalysis and corrosion. As a prototype example, we consider one of the most corrosive systems under wet conditions - Mg. Using the new approach we solve a 150-year-old problem, which links H-evolution under anodic conditions to Mg dissolution [1].

[1] S. Surendralal, M. Todorova, M.W. Finnis and J. Neugebauer, Phys. Rev. Lett. 120, 246801 (2018).

CPP 36.3 Wed 11:30 H9

Towards out of the box implicit solvation at liquid-liquid interfaces — •Jakob Filser[1], Markus Sinstein[1], Christoph Scheurer[1], Sebastian Matera[2], Karsten Reuter[1], and Harald Oberhofer[1] — [1]Technische Universität München — [2]Freie Universität Berlin

Implicit solvation models are widely used to incorporate solvent effects in electronic structure theory. Treating the solvent as a structureless dielectric continuum, they lift the necessity to explictly sample solvent degrees of freedom. However, even state of the art models currently cannot treat solvation at technically highly important dielectric interfaces, e.g. between two immiscible liquids.

As a remedy, we modify the multipole expansion (MPE) model to also account for liquid-liquid interfaces, specifically focusing on the electrostatics of mutually interacting dielectric regions. Non-electrostatic free energy contributions thereby are treated with a simple linear model, fitted to experimental free energies of solvation in the two liquids. We demonstrate the efficacy of this approach for small molecules at a water–1-octanol interface, which show the correct qualitative behaviour with respect to orientation and position at the interface.

Future, quantitative applications of our new implicit solvation interface methods are clearly possible but will necessitate both improvements to the non-electrostatic free energy terms and a more exhaustive parameterization effort for a wide range of solvents.

CPP 36.4 Wed 11:45 H9

Continuum models of the electrochemical diffuse layer in electronic-structure calculations — •Francesco Nattino[1], Oliviero Andreussi[2], and Nicola Marzari[1] — [1]Theory and Simulations of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — [2]Department of Physics, University of North Texas, Denton, TX 76207, USA

The electrical diffuse layer is a structure that spontaneously forms at essentially any solvated interface, such that its presence in electrochemistry is ubiquitous. While first-principles methods are desirable to describe any process occurring at the surface, fully-atomistic models of electrolyte solutions suffer from computational limitations. In this context, continuum models represent a practical tool to bypass these difficulties and to account for the presence of the diffuse layer at electrified interfaces. However, despite the increasing popularity of continuum models in the field of materials science, even relatively simple observables such as the differential capacitance (DC) of single-crystal electrode surfaces remain challenging to model quantitatively. I will present and discuss the performance of a hierarchy of continuum diffuse-layer models that we have implemented and coupled to an atomistic first-principles description of a charged metal surface. In particular, I will compare computed DC values for the prototypical Ag(100) surface in an aqueous solution to experimental data, and validate in this way the accuracy of the models considered.

CPP 36.5 Wed 12:00 H9

***Ab initio* molecular dynamics of Pt(111)/H_2O interfaces in an electrolytic cell setup** — •Sudarsan Surendralal, Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany.

Recently, we developed a novel scheme to perform density functional theory (DFT) simulations of electrochemical interfaces under conditions of constant applied voltage utilizing charge transfer from a semiconductor counter electrode [1]. We use a fractionally doped Ne counter electrode because of its inertness, wide band gap, and low deformation potential. Our DFT based molecular dynamics calculations of the Pt(111)/H_2O interface in this setup reveals that we are able to accurately reproduce macroscopic observables like the potential of zero charge (PZC). We discuss the work function drop at the interface at the PZC, due to the charge polarization by the non-dissociative chemisorption of water molecules at the Pt surface. Possible pitfalls due to the choice of the DFT exchange-correlation functional, non-converged computational parameters and confinement effects due to the presence of the counter electrode will also be discussed.

[1] S. Surendralal, M. Todorova, M. W. Finnis, and J. Neugebauer, Phys. Rev. Lett. 120, 246801 (2018).

CPP 36.6 Wed 12:15 H9

Swipe left for water molecules? - Implicit vs explicit descriptions of liquid water at interfaces. — •Nicolas Hörmann[1], Oliviero Andreussi[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), EPFL, CH-1015 Lausanne, Switzerland — [2]Department of Physics, University of North Texas, Denton, TX 76207, USA

We present a study of relevant electrochemical interfaces, such as semiconductor-water and metal-water interfaces based on periodic density functional theory (DFT) calculations with the interface modelled with different degrees of complexity. Water at metallic surfaces is modelled within the self-consistent continuum solvation scheme (SCCS) [1] with explicit application of a potential which allows the comparison of pH dependent properties with experimental results [2,3]. In the case of semiconductors, different amounts of interfacial water are substituted with implicit solvent and observables such as the measured band alignment are obtained from thermal averaging over molecular dynamics snapshots. We find that it is necessary and sufficient to include strongly bound interfacial water molecules (dissociated or not) explicitly and replace the rest with an implicit model, in order to obtain consistent results with all-explicit simulations [4]. Based on these result we simulate the surface Pourbaix diagrams of the most stable surfaces of GaAs, GaN, GaP, CdS and anatase and rutile TiO_2.

[1] *J. Chem. Phys.* **136**, 064102 (2012); [2] *Nat Commun.* **9**, 3117 (2018). [2,3] NH (2018) submitted

CPP 36.7 Wed 12:30 H9

Transition metal oxide nanoparticles as efficient catalysts for proton exchange membrane electrolyzers: morphology, activity and stability — •Daniel Opalka, Yonghyuk Lee, Jakob Timmermann, Christoph Scheurer, and Karsten Reuter — Technische Universität München

Transition metal oxides such as RuO_2 and IrO_2 are currently the best known electrocatalysts for the oxygen evolution reaction from liquid water in proton exchange membrane (PEM) electrolyzers. However, dynamic load operation of PEM cells induces transformations of the catalyst morphology leading to metal dissolution and catalyst degradation. We present a computational model to predict the morphology, activity and stability from *ab initio* electronic structure theory and fundamental thermodynamic principles. Based on this model, we have explored novel strategies to reduce material expenses and improve catalyst stability while preserving high catalytic activity via nanoparticles with a core-shell design. From an analysis of different surface coverages with oxygen, hydroxyl and hydroxo species, voltage-dependent phase diagrams for catalyst surfaces are presented which correlate with characteristic features observed in cyclovoltammetric measurements. Results from atomistic models of selected nanoparticles on the basis of Wulff's Theorem show negligible size effects, but a strong influence of the facet terminations on the surface relaxation.

CPP 36.8 Wed 12:45 H9

Modelling the fingerprint of chemical reactions on catalytic surfaces in core-electron binding energies — •Johannes Lischner and Juhan Matthias Kahk — Imperial College London

Core-electron X-ray photoemission spectroscopy is a powerful experimental technique to gain information about chemical reactions on catalytic surfaces. Interpreting experimental spectra, however, is often challenging and theoretical modelling of core-electron binding energies is required to meaningfully assign peaks to adsorbate species. In this talk, I will present a novel first-principles modelling strategy to calculate core-electron binding energies of molecules on metallic surfaces. Specifically, we combine plane-wave/pseudoptential DFT calculations of surface slab models for geometry optimizations with all-electron Delta-SCF calculations on cluster models for determining accurate core-electron binding energies. This approach is computationally efficient and yields good agreement with experimental measurements for a wide range of adsorbates on copper(111) surfaces.

CPP 36.9 Wed 13:00 H9

What Makes a Successful Photoanode? - The Role of the Semiconductor–Catalyst Interface — •Franziska Simone Hegner[1], Benjamin Moss[2], James Durrant[2], Sixto Gimenez[3], José-Ramón Galán-Mascarós[1], and Núria López[1] — [1]Institute of Chemical Research of Catalonia (ICIQ) — [2]Imperial College London — [3]Institute of Advanced Materials, Castellón

A large scale implementations of artificial photosynthesis is still limited by the low efficiencies of the employed photoelectrochemical systems. A common strategy to improve performance is to deposit a co-catalyst on the light-harvesting photoanode. However, the role of the catalyst is controversial; is it acting as a true catalyst, i.e. transferring charges, or is it merely influencing the electronic structure of the semiconductor?[1]

The semiconductor-catalyst interface is key to catalytic performance, but its accurate description is limited since linear scaling relationships no longer apply. Herein the function of the co-catalyst (cobalt hexacyanoferrate) is discussed on two photoanode interfaces, Fe2O3 and BiVO4. Density Functional Theory and time-resolved spectroscopy were used to shed light on the underlying charge-transfer processes. Taking into account the advantages and disadvantages of all applied techniques, a relationship between electronic structure alignment, interface morphology, and photocatalytic efficiency is proposed.[2]

[1] D. R. Gamelin, Nat. Chem., 4 (2012), 965-967. [2] F. S. Hegner, D. Cardena-Moscoros, S. Gimenez, N. López, J. R. Galán-Mascarós. ChemSusChem, 10 (2017) 4552-4560.

CPP 37: Poster Session III

Topics: Controlling Phase Formation Dynamics in Solution Processed Semiconductors (37.1-37.4); Hybrid and Perovskite Photovoltaics (37.5-37.17); Molecular Electronics and Excited State Properties (37.18-37.23); Organic Electronics and Photovoltaics (37.24-37.55).

Time: Wednesday 11:00–13:00 Location: Poster B1

CPP 37.1 Wed 11:00 Poster B1

Key factors in the synthesis of template-oriented porous ordered titanium dioxide: solvents and catalysts — •Shanshan Yin and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

As a crucial material for energy storage, TiO2 has been widely studied during the past decades. Typically, when used as the active material of lithium-ion batteries or solar cells, TiO2 thin films with specific structures always afford more advantages than classical bulk material. In this work, various intriguing structures have been synthesized with the template-oriented sol-gel method. Both, the hydrolysis and condensation reaction of TTIP, are confined into the PEO domain of the amphiphilic diblock copolymer during the sol-gel synthetic process. Since the polymer template can be fully removed with the calcination, the morphology control of the TiO2 thin film is realized with controlling the phase separation behavior of the block polymer. In the present work, the influence of the solvent category and catalyst content on the morphology of TiO2 thin film is discussed in detail. SEM and GISAXS measurements were carried out to study the pore structures of the TiO2 films.

CPP 37.2 Wed 11:00 Poster B1

Ordering and crystallization in thin films of diketopyrrolopyrrol-based semiconducting copolymers — •Shayan Vazirieh Lenjani, Mario Zerson, Qian Wang, Michael Sommer, and Robert Magerle — Fakultät für Naturwissenschaften, TU Chemnitz, Chemnitz, Germany

Semiconducting polymers based on diketopyrrolopyrrol (DPP) combine a number of favorable properties, such as straightforward chemical synthesis and photostability with an outstanding charge carrier mobility in organic electronic devices. Despite this success, the structure formation processes in thin films are poorly understood. With atomic force microscopy (AFM), we study thin films of DPP copolymers prepared from different solvents, polymer concentrations, and temperatures. During drying, a complex sequence of structural rearrangement processes occurs. In solution, the polymers partly form aggregates. At higher polymer concentrations, different types of lyotropic liquid crystalline phases form as indicated by terrace formation and the observed surface textures. During the final drying, the polymer chains partly crystallize and form crystalline lamellae that are typical for semicrystalline polymers. From arrays of pointwise measured amplitude–phase–distance curves, we reconstruct three-dimensional depth profiles of the specimen's top 10 nm surface layer. These high-resolution volume images reveal different types of surface structures with unprecedented resolution.

CPP 37.3 Wed 11:00 Poster B1

What is the role of planarity and torsional freedom for aggregation in organic semiconductor materials? — •Stefan Wedler[1], Axel Bourdick[2], Stephan Gekle[2], Fabian Panzer[1], Caitlin McDowell[3], Guillermo C. Bazan[3], Thuc-Quyen Nguyen[3], and Anna Köhler[1,4] — [1]Soft Matter Optoelectronics, University of Bayreuth — [2]Biofluid Simulation and Modeling, University of Bayreuth — [3]Center for Polymers and Organic Solids, UC Santa Barbara — [4]BIMF, University of Bayreuth

Planarity and rotational freedom play an important role for the aggregation process in organic semiconductors. Stiff and planar molecules seem to aggregate more easily. However, it is not clear whether these factors are a prerequisite or just a side effect of aggregation. We investigate the importance of planarity for aggregation using two small conjugated molecules, which consist of typical building blocks and differ only by the rigidity of their central unit. Their aggregation properties are compared by absorption and luminescence spectroscopy, both temperature dependent in solution as well as in-situ upon spincasting during film formation. MD simulations and DFT calculations reveal intermolecular arrangements. Our results suggest that planarity and torsional rigidity are indeed needed to promote aggregation, though too much rigidity can obstruct the pathway to ordered structures.

CPP 37.4 Wed 11:00 Poster B1

Investigating the Role of Planarity and Torsional Freedom for Aggregation in Organic Semiconductor Materials with the Help of MD and DFT Simulations — Stefan Wedler[1], •Axel Bourdick[2], Stephan Gekle[2], Fabian Panzer[1], and Anna Köhler[1] — [1]Experimental Physics II, University of Bayreuth — [2]heoretical Physics VI , Biofluid Simulation and Modeling, University of Bayreuth

Organic photovoltaics has become a rapidly developing field, in which a lot of interesting systems are investigated for potential industrial applications. An ongoing challenge hereby is to relate the aggregation to the macroscopic properties of the solar cells. Planarity and rotational freedom play an important role during the aggregation process but the details of the mechanism is poorly understood. We use MD and DFT simulations to gain insights at molecular length scales which is difficult to access by experiments alone. We investigate two small conjugated molecules with a tandem like design structure, which differ in the planarity of the central donor units. The aggregation properties are investigated by optical experiments (presented on the accompanying poster by S. Wedler et al [1]), which we support with simulations. Free energy calculations and an investigation of the properties of the aggregates lead to a better understanding of the importance of planarity and rotational freedom.

[1]: Poster, What is the role of planarity and torsional freedom for aggregation in organic semiconductor materials?, S. Wedler et. al.

CPP 37.5 Wed 11:00 Poster B1

Water-processed active layers for hybrid photovoltaics using spray deposition techniques — •Lautaro Díaz Piola, Volker Körstgens, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Hybrid solar cells aim to combine the advantages of both, inorganic and organic materials in the active layer. The stability and high carrier mobility of the inorganic component, together with the potential low-cost production and feasibility of producing flexible devices from the organic component make the hybrid approach promising. In particular, the possibility for wet chemical device preparation in the organic material allows the use of scalable thin film coating techniques. Most of the research in this direction use organic solvents for the solar cell preparation, which does not lead to a full environmentally friendly approach. Therefore, the use of water soluble components for the organic material is of interest. In the present investigation we study the morphology of active layers for hybrid solar cells that are fully water processed using industrially scalable techniques such as spray coating. The investigation of the mesoscale structure and of the crystal structure is carried out via the scattering techniques GISAXS and GIWAXS, respectively, while UV/vis measurements are performed to study the absorption properties.

CPP 37.6 Wed 11:00 Poster B1

Impact of microstructure of hybrid perovskite powders on the mechanical properties of completely dry processed perovskite layers via pressing — •Maximilian Schultz[1], Nico Leupold[2], Konstantin Schötz[1], Ralf Moos[2], and Fabian Panzer[1] — [1]Soft Matter Optoelectronics — [2]Department of Functional Materials, all University of Bayreuth, Bayreuth, 95440, Germany

Optoelectronic devices based on hybrid perovskites have undergone a remarkable development within the last few years. However, state of the art processing approaches such as solution processing or evaporation suffer from an intrinsically high complexity, as the actual perovskite crystallization and its film processing happen simultaneously and are inextricably interconnected.

Here we present an alternative, entirely dry processing approach, which decouples perovskite crystallization and film formation, by using readily prepared perovskite powders and produce films by appropriate mechanical pressure treatment. We show how the used pressure and the powder microstructure, i.e. particle size and stoichiometry affect the mechanical stability, compactness and surface roughness of the pressed layers. We further address how specific temperature treatment during the pressing step can be used to improve the properties of the pressed layer.

CPP 37.7 Wed 11:00 Poster B1

The 2-Step deposition method of mixed perovskites as a route to highly tunable optoelectronic properties — •Lennart Reb and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Mixed-cation lead mixed-halide perovskite solar cells with their impressive increase in efficiency over the last years, exceeding 22 per cent recently, are promising to play a role for future and sustainable power generation. Typically, the well-established 1-step spin-coating deposition technique is used for the perovskite layer to achieve these high efficiencies. In contrast, the 2-step deposition technique takes full advantage of the chemical tuneability of the perovskite semiconductors. Probing such perovskite thin films of different chemical compositions and concentrations with grazing incidence small- and especially wide-angle X-ray scattering allows assessing their morphological and crystalline structure. Spectroscopic measurements, e.g. ellipsometry, external quantum efficiency measurements, impedance spectroscopy, complement the structural investigations and thereby help us to increase our knowledge of some still poorly understood physical mechanisms in perovskite solar cells. More importantly, this is a necessary step to be able to tune the fascinating optoelectronic properties of perovskite to access the full range of other promising applications, such as photo-detectors and light emitting diodes.

CPP 37.8 Wed 11:00 Poster B1

Characterization and Encapsulation of Perovskite Solar Cells — •Benjamin Predeschly, Lennart Reb, and Peter Müller-Buschbaum — TU München, Physik Department, LS Funktionelle Materialien, 85748 Garching, Germany

Perovskite Solar Cells (PSCs) with their upscalable low-cost production from solution and their flexibility, suited for new application fields, are promising for future energy generation. Impressive power conversion efficiency (PCE) of more than 20 percent was reached recently as a result of optimized preparation techniques and material compositions. However, PSCs exposed to ambient conditions, especially humidity, show a decreasing PCE with time, making long-term stability a bottleneck towards commercialization. We process PSCs with the champion architecture and investigate them by various methods like external quantum efficiency measurements, scanning electron microscopy and grazing incidence small- and wide-angle X-ray scattering (GISAXS and GIWAXS) to relate the morphological changes to the degradation of the device performance. To improve the long-term stability, we develop a simple but effective method for mechanical encapsulation, protecting the PSC with a flexible foil from humidity. We track the PCE of the encapsulated PSCs over time, with a substantial improvement of the long-term stabilization in ambient condition, which is supported by GIWAXS measurements. Reaching long-term stability for PSCs is an important step towards their success.

CPP 37.9 Wed 11:00 Poster B1

Mesoporous Titania Backfilled with Heavy Element Containing Small Molecules and High-Efficiency Polymer PTB7-Th for Hybrid Photovoltaics — •Raphael Märkl[1], Nuri Hohn[1], Emanuel Hupf[2], Gaetano Mangiapia[3], Matthias Pomm[3], Eric Rivard[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]University of Alberta, Department of Chemistry, Edmonton, Canada — [3]Helmholtz-Zentrum Geesthacht at Heinz Maier-Leibnitz Zentrum, Garching

Hybrid photovoltaic devices have recently attracted significant research attention due to improvements in efficiency by tailoring the organic-inorganic interface. Mesoporous titania films are synthesized utilizing polystyrene-b-polyethyleneoxide diblock copolymer templating in a sol-gel approach. A hybrid photovoltaic active layer is then achieved by infiltrating the organic component into the resulting mesoporous titania scaffold. We investigate the backfilling of organic polymer PTB7-Th and novel tellurophene Phen-Te-BPinPh small molecule into the mesoporous titania films by ToF-GISANS. While the backfilling efficiency of PTB7-Th proves to be sensitive to the polymer concentration, Phen-Te-BPinPh is backfilled easily into the titania matrix due to its small size. Complementary X-ray scattering techniques are used in obtaining the SLD profile required for ToF-GISANS analysis and the crystal structure of respective thin films. Conclusions derived from real space investigation via SEM are found in agreement with these results.

CPP 37.10 Wed 11:00 Poster B1

Comparative study of interface modification and passivation approaches on low-temperature SnO2 and their effect on perovskite solar cell performance — •Max Grischek, Philipp Tockhorn, Ganna Chistiakova, Lukas Kegelmann, and Steve Albrecht — Helmholtz-Zentrum Berlin, Berlin, 12489, Germany.

SnO2 is a widely used electron transporting material (ETM) in planar n-i-p-type perovskite solar cells (PSC). It allows high Voc above 1.15 V and efficiencies close to 21%. In addition, low process temperatures make SnO2 a suitable ETM for flexible foils or monolithic silicon-perovskite tandem solar cells. However, high device efficiencies require thorough optimization of the SnO2 surface. This study investigates modification and passivation approaches on SnO2 and compares their effect on chemical composition, energetics, charge carrier extraction, interface recombination and performance in PSCs. Firstly, a dipole interlayer between SnO2 and the absorber is utilized to reduce the SnO2 workfunction and its conduction band offset to the absorber, as implied by UPS. This is shown to reduce interface recombination losses and increase the device Voc, as revealed by absolute PL and J-V measurements. Similar effects are observed when introducing very thin interlayers of PCBM/PMMA mixtures. The best PSC performance is achieved by an O2-plasma treatment of the SnO2 surface. Using J-V, TRPL and absolute PL measurements, less non-radiative recombination and faster charge carrier extraction are observed. This plasma treatment leads to reduced hysteresis and an enhancement in device efficiency to 18.1%.

CPP 37.11 Wed 11:00 Poster B1

Preparation of $Mg_xZn_{1-x}O$ nanoparticles through a wet chemical route for applications in optoelectronic devices — •Andreas Ringleb and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik

Zinc oxide (ZnO) is an n-type semiconductor and a promising candidate for applications in various types of optoelectronic devices due to its wide direct bandgap of about 3.3 eV and high exciton binding energy of approximately 60 meV. The targeted substitution of Zn with magnesium enables a tunable band gap of $Mg_XZn_{1-X}O$ between 3.3 and 7.8 eV through control of the Mg-content. $Mg_XZn_{1-X}O$ nanoparticles have been prepared from acetate precursors through a wet chemical route. Thin films have been deposited on quartz and FTO coated glass substrates from pastes by doctor-blading and subsequent drying and/or annealing. XRD and SEM have been used to study the morphology and crystal structure of these films. The modulation of the band gap has been confirmed by UV-Vis spectroscopy. Elemental composition has been studied by XPS and EDX. Nanoparticle size has been measured by means of dynamic light scattering (DLS). A focus has been put on the homogeneity and porosity of the resulting films since they are especially suited for future applications in hybrid photovoltaics, such as dye-sensitized solar cells (DSCs), quantum-dot solar cells (QDSCs) or perovskite solar cells (PSCc).

CPP 37.12 Wed 11:00 Poster B1

Time-Resolved Microwave Conductivity on Lead Halide Perovskite Films — •Patrick Dörflinger[1], Andreas Baumann[2], Andreas Sperlich[1], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Perovskite solar cells are one of the most promising new photovoltaic technologies with steadily rising efficiencies. To further improve their potential performance and stability, it is essential to understand their optoelectrical properties as well as to develop novel, not yet established, perovskite materials. These must be extensively characterized prior to solar cell fabrication. With Time-Resolved Microwave Conductivity (TRMC) the mobility and lifetime of photogenerated charge carriers in a perovskite layer can be determined in a non-contact way. The TRMC measurement technique is based on the interaction of an applied electro-magnetic field with the charge carriers in the semiconductor material, which leads to a time-dependent change in conductance. We use TRMC to probe the charge carrier dynamics in various perovskite materials, such as methylammonium lead iodide and mixed cation and halide perovskite.

CPP 37.13 Wed 11:00 Poster B1

Influence of Ammoniumvaleric Acid on the Current-Voltage Hysteresis of $MAPbI_3$ Thin Films on Microstructured Electrode Arrays — •Jonas Glaser, Jonas Horn, Raffael Ruess, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik

As organic-inorganic lead halide perovskite solar cells have emerged as promising technology for low-cost and highly efficient photovoltaics, issues such as long term stability and hysteresis in the current-voltage characteristics are put into focus of interest. Microstructured metal electrode arrays can be used to investigate electrical and interface properties of such semiconducting layers. In this work, thin films of methylammonium lead iodide ($MAPbI_3$) were prepared on microstructured platinum arrays in order to study the I-V-characteristics under different applied voltages. Partial substitution of methylammonium by ammoniumvaleric acid was found to reduce the observed hysteresis and, also, decreased the measured current densities by about one order of magnitude. It was found that the appearance of the hysteresis strongly depends on the chosen measurement conditions, e. g., scan rate and voltage range. Therefore, we assume that the application of an external electric field leads to alignment of dipoles and migration of ions and vacancies in the perovskite thin films, which then shows two kinds of I-V-hysteresis, one for smaller voltages that is not influenced by the scan rate and another one for larger applied electric fields whose extent depends on the scan rate.

CPP 37.14 Wed 11:00 Poster B1

Electrical Characterization of the Double Perovskite $Cs_2AgBiBr_6$ — •Fabian Schmitz, Jonas Horn, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik

Hybrid organic-inorganic lead halide perovskites have been investigated intensively during the last decade. Issues of chemical stability, interfacial contact formation and the toxicity of lead represent the main present challenges for perovskite solar cells. Fully inorganic absorbers, such as the double perovskite $Cs_2AgBiBr_6$ provide a possible solution to some of these problems. Despite rather fast nongeminate recombination, this material is not only a promising approach to overcome the stability issues but also facilitates ambient processing with less problematic solvents and reduces the toxicity problems of prospective cells.[1] We prepared such inorganic layers to evaluate their suitability as absorber or buffer layers in solar cells by measuring their I-V-characteristics in the dark and under illumination, incident photon conversion efficiency and open circuit voltage decay. Further, we measured the electronic properties of $Cs_2AgBiBr_6$ layers using symmetric metal contacts in order to investigate I-V-hysteresis, which is a good indicator of contact characteristics in perovskite solar cells.

[1] R. Kentsch, M. Scholz, J. Horn, D. Schlettwein, K. Oum, T. Lenzer, *J. Phys. Chem. C*, **122**, 25940 (2018).

CPP 37.15 Wed 11:00 Poster B1

Charge Carrier Dynamics of the Double Perovskite Cs$_2$AgBiBr$_6$ — •Robin Kentsch[1], Mirko Scholz[1], Jonas Horn[2], Derck Schlettwein[2], Kawon Oum[1], and Thomas Lenzer[1] — [1]Physikalische Chemie, Universität Siegen, Adolf-Reichwein-Str. 2, 57076 Siegen, Germany — [2]Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Hybrid lead perovskites have reached power conversion efficiencies above 23% in photovoltaic applications. Yet, major drawbacks remain. These include the toxicity of lead as well as the insufficient long-term stability. The ongoing search for environmentally friendly alternatives has identified so-called "double perovskites" with the general formula A$_2$MM'X$_6$ as potential replacements. Here, we report results for the charge carrier dynamics of the lead-free silver-bismuth double perovskite Cs$_2$AgBiBr$_6$ by employing time-resolved optical spectroscopy and electrical measurements.[1] Upon photoexcitation, we identify fast charge carrier cooling processes and pronounced coherent oscillations in the picosecond range. This is consistent with strong electron-phonon coupling. Furthermore, excitonic contributions are found. Electron-hole recombination occurs in the time range from several hundred picoseconds to microseconds. Implications of this charge carrier dynamics for the energy conversion efficiency of this lead-free perovskite in the real device will be discussed.

[1] R. Kentsch, M. Scholz, J. Horn, D. Schlettwein, K. Oum, T. Lenzer, *J. Phys. Chem. C*, **122**, 25940 (2018).

CPP 37.16 Wed 11:00 Poster B1

Unravelling the origin of double peak emission of hybrid perovskites — •Konstantin Schötz[1], Abdelraham Askar[2], Wei Peng[3], Dominik Seeberger[1], Tanaji P. Guijar[1], Mukundan Thelakkat[1], Sven Hüttner[1], Osman Bakr[3], Karthik Shankar[2], Anna Köhler[1], and Fabian Panzer[1] — [1]University of Bayreuth, 95440 Bayreuth, Germany — [2]University of Alberta, Edmonton, AB T6G 1H9, Canada — [3]King Abdullah University of Science and Technology (KAUST), Thuwal23955-6900, Kingdom of Saudi Arabia

The optical properties of hybrid perovskites are known to be sensitively interconnected with their structure, which is soft and thus prone for changes. Double photoluminescence (PL) peaks have been reported at low temperatures, and recently also at room temperature, though there is still no consensus about the origin of this double PL peak structure. Here we show that the occurrence of the additional PL peak is not limited to one specific material composition and that it occurs in single crystals as well as in thin films, rendering it a general phenomenon. We systematically investigate the origin of this additional PL feature by measuring and analyzing temperature-dependent one- and two-photon-induced PL. Together with fluence dependent measurements, optical modelling and systematic surface treatments, we can differentiate the impact of various possible physical and optical effects such as e.g. self-absorption, excited state diffusion or surface states, in order to gain a detailed and elaborated understanding on the occurrence of multiple PL peak phenomena in hybrid perovskites.

CPP 37.17 Wed 11:00 Poster B1

Using polymeric hole-injection layers for solution-processed Perovskite-based light-emitting diodes — •Tassilo Naujoks[1], Thomas Morgenstern[1], Manuel Engelmayer[1], Matthew Jurow[2], Yi Liu[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States of America

Replacing common organic emitters with Lead-Halide Perovskites, like CsPbBr$_3$, is a promising approach towards low cost, efficient and narrow emission-band LEDs. While showing high photoluminenscent quantum-yields in thin films [1], achieving similarly high performance in elec devices proves to be challenging. Protection of the hole injection layer either by shielding films or orthogonal solvents has a huge effect on the optoelectronic properties. A hole-injection layer for a solution-processed emitter should not be impaired by the respective solvent. Such films can be formed by crosslinked polymers.

In this study we investigate the synergy of poly-TPD as hole-injection polymer and CsPbBr$_3$ quantum dots as emitter in an otherwise common organic LED stack. Furthermore the use of different polymers or combinations show significantly increased efficiency. The efficiency proves to be correlated to the respective solvent susceptibility of the layers. The findings are of huge importance for future applications of lead-halide perovskites in optoelectronic lighting applications.

[1] Becker, Michael, *et. al.* Nature **553**, 189 (2018)

CPP 37.18 Wed 11:00 Poster B1

p-type doping of organic semiconductors with polycyclic acceptors — •Adriana Röttger[1], Berthold Wegner[1], Andreas Opitz[1], and Norbert Koch[1,2] — [1]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

Predictions about ion pair formation (IPA) of organic donor/acceptor blends can be made based on redox-potentials measured by cyclic voltammetry in solution or based on ionisation energies (IE) / electron affinities (EA) measured on thin films by direct / inverse photoelectron spectroscopy. Here, we investigate the accuracy of these predictions for two different organic semiconductor systems in solutions and thin films. At first optical absorption spectroscopy is employed to determine IPA yield in mixtures of two pyrene derivatives as donors and three polycyclic acceptors, which exhibit similar chemical structures. Since the predictions from redox potential and IE/EA do not differ significantly, both prove accurate. The second system consists of the polymer P3HT doped with the same set of acceptors. Again, optical absorption spectroscopy was used to determine the presence of ionic molecular species as well as formed polarons in P3HT. These predictions also prove accurate. In addition, scanning force microscopy and current-voltage measurements were performed to examine the impact of doping on surface morphology and electrical conductivity of P3HT films, respectively.

CPP 37.19 Wed 11:00 Poster B1

Ultrafast photophysics of TIPS-tetracenophane — •Clemens Zeiser[1], Andreas Göttler[2], Luca Moretti[3], Margherita Maiuri[3], Giulio Cerullo[3], Tetsuhiko Nagahara[3,4], Holger F. Bettinger[2], and Katharina Broch[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]Institut für Organische Chemie, Universität Tübingen, Germany — [3]Dipartimento di Fisica, Politecnico di Milano, Italy — [4]Department of Chemistry and Materials Technology, Kyoto Institute of Technology, Japan

Singlet exciton fission is a process which could help to improve the power-efficiencies of silicon solar cells by providing a solution to overcome the Shockley-Queisser-Limit. Tetracene is one of the most promising compounds for application as a singlet fission layer [1] and its photophysical properties thus need to be well understood. Chemically linked tetracene dimers [2] provide an opportunity to alter the relative orientation of two tetracene monomers and, thus, to study its influence on the singlet fission time constant. Here we report on the photophysics of the linked TIPS-tetracene dimer TIPS-tetracenophane (TIPS-TCP) [3], where the two tetracene monomers are doubly linked and facing each other directly. Using transient absorption spectroscopy on thin films of TIPS-TCP, we find a singlet lifetime significantly longer than that of tetracene and interpret this finding as an ultrafast creation of a triplet pair state, but a hindered separation of the two triplets.

[1] R. W. MacQueen et. al., *Mater. Horiz.* **5** (2018) [2] N. V. Korovina et. al., *J. Am. Chem. Soc.* **140** (2018) [3] H. F. Bettinger et. al., *Org. Chem. Front.* **4** (2017)

CPP 37.20 Wed 11:00 Poster B1

Ab initio many-body study of the electronic structure of the Lewis acid Tris(pentafluorophenyl)borane (BCF) — •Richard Schier, Ana M. Valencia, and Caterina Cocchi — Physics Dept., Humboldt-Universität zu Berlin und IRIS Adlershof

Doping in organic semiconductors is an attractive area of research for molecular electronics. The Lewis-acid tris(pentafluorophenyl)borane (BCF)[1] is a strong electron acceptor already successfully employed as a p-dopant in organic semiconductors[2]. However, a clear understanding of its electronic structure is still missing. We fill this gap in a first-principles study based on density-functional theory with hybrid functionals and many-body perturbation theory, including the GW approximation, as implemented in the MOLGW code[3]. For comparison, we relate BCF to its building block hexafluorobenzene (C6F6).

For BCF, we find that both the LUMO and the HOMO are non-degenerate. The LUMO is mainly localized around the boron atom, consistent with the electron-withdrawing character of this molecule. On the other hand, the HOMO is distributed only on the phenyl-rings without any participation of the boron. From GW, the HOMO energy of BCF and C6F6 differs by about 250 meV, suggesting that these two molecules have approximately the same ionization potential.

[1] Körte et al., Angew. Chem. 56, 8578 (2017) [2] Pingel et al., Adv. Electron. Mater. 2, 1600204 (2016) [3] Bruneval et al., Comput. Phys. Commun. 208, 149 (2016)

CPP 37.21 Wed 11:00 Poster B1

The statistics of photoluminescence quantum yield measurements — •Felix Fries, Heidi Thomas, Max Gmelch, Tim Achenbach, and Sebastian Reineke — IAPP, Technische Universität Dresden, 01187 Dresden, Germany

Measuring the photoluminescence quantum yield (PLQY) is both a well-known and often used method within many different fields of luminescent materials. Knowing a material's PLQY not only allows estimating its use for applications but also gives further insights into the physics within. Calculating the radiative rate of a fluorescent decay is only one of many examples. The common setup comprises a light-source for excitation, an integrating sphere, and a spectrometer or photodiode for signal detection. However, to assure accurate results the measurement relies on a very stable light source.

Here we show that even with low cost devices as LEDs, reliable values with a low statistical error can be obtained. Therefore, we investigate the importance of a right statistical treatment of the measured data. Furthermore, sources of systematic errors in the setup can easily be detected that way.

Evaluating the results of PLQY measurements on solid-state samples of organic molecules showing both fluorescent and phosphorescent emission at room temperature (biluminescence), we are able to deduce information about the singlet's and triplet's PLQY separately and also about intermolecular interaction processes like singlet-triplet annihilation.

CPP 37.22 Wed 11:00 Poster B1

Molecular design of λ^6-phosphorus compounds for OLED applications — •Juliana Nair, Jonas Köhling, Gerd-Volker Röschenthaler, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Organic light emitting diodes (OLEDs) are one of the leading technologies used as active optoelectronic device in displays. Currently, in OLED displays the most challenging quest is to synthesize and design efficient and stable blue emitters. To achieve this goal it is of great interest to evaluate possible molecules prior to synthesis and to optimize their molecular design.

In this study a large amount, i.e. 151 derivatives, of λ^6-phosphorus fluorescent compounds were evaluated regarding their light emitting properties. As basic structure the central phosphorous atom is bound to one derivative of 8-Quinolinol as well as 4 Fluorine atoms. 8-Quinolinol was systematically varied by introduction of substituents from strong electron withdrawing groups (EWG) towards strong electron donating groups (EDG). Besides the mesomeric and inductive electron withdrawing and donating effects also the position of the substituent has a crucial influence on the calculated emitting wavelength of these fluorophores. To determine the emitting wavelength of an isolated molecule time-dependent density functional theory (B3LYP/6-31+G(d,p)) was employed. EWGs tend to increase the bandgap if placed on the benzene ring of the ligand, where EDGs show the same effect when substituted on the pyridine ring of the ligand. This allows to tune the calculated bandgap between 3.2 - 4.1 eV.

CPP 37.23 Wed 11:00 Poster B1

Micro-Refractometry and Local-Field Mapping with Single Molecules — Andrei V. Naumov[1,2], Alexey A. Gorshelev[1], Maxim G. Gladush[1,2], Tatiana A. Anikushina[1,2], Alina V. Golovanova[1,2], Jürgen Köhler[3,4,5], and •Lothar Kador[3] — [1]Institute for Spectroscopy, Russian Academy of Sciences, Moscow 108840, Russia — [2]Moscow State Pedagogical University, Moscow 119435, Russia — [3]University of Bayreuth, Institute of Physics, 95440 Bayreuth, Germany — [4]University of Bayreuth, Spectroscopy of Soft Matter, 95440 Bayreuth, Germany — [5]Bavarian Polymer Institute, 95440 Bayreuth, Germany

Single-molecule spectroscopy at cryogenic temperatures was used to measure and map the local index of refraction in a solid with nanometer resolution. The natural zero-phonon linewidth of 1950 single terrylene molecules in a matrix of polycrystalline *n*-hexadecane was measured at $T = 1.5$ K where thermal broadening effects are absent. The linewidth is then determined by the excited-state lifetime which depends on the local density of states of the electromagnetic field, i.e., the local refractive index. The spatial resolution is on the order of a few nanometers; it is given by the accuracy with which fluorescing single molecules can be localized. Unexpectedly large fluctuations of the local refractive index between 1.1 and 1.9 were found. Three different distance ranges could be roughly identified, in which the fluctuations have different magnitudes.

CPP 37.24 Wed 11:00 Poster B1

Voltage-dependent shift of the emission spectra of exciplex OLEDs — •Thomas Schröther, Thomas Zechel, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Exciplexes are excited states between two different molecules in an organic light emitting diode (OLED). After electrical excitation, the hole is located in the highest occupied molecular orbital (HOMO) of the donor material and an electron occupies the lowest unoccupied molecular orbital (LUMO) on the acceptor. These states are recently used to improve the external quantum efficiencies in OLEDs.

In this work we investigated the electroluminescence spectra of the material combination m-MTDATA:BPhen forming exciplex states in OLED devices using two layouts, where the molecules were either mixed or in separate planar layers. After varying the applied voltage, it was possible to discern between two different kinds of spectral shifts that depend on the layout by fitting the data with multiple Gaussian functions. In the mixed OLED the positions of the individual peaks are constant but their contribution to the emission changes. Whereas every single Gaussian shifts with constant height in the planar device resulting in a shift of the whole curve. Based on the theoretical description by Monkman and Al Attar [1] as well as Linderl [2], we present two models to explain this observed difference.

[1] H. A. Al Attar, A. P. Monkman, *Adv. Mat.* 28 (36), 8014 - 8020 (2016), DOI: 10.1002/adma.201600965

[2] T. Linderl, PhD thesis, University of Augsburg (2017).

CPP 37.25 Wed 11:00 Poster B1

Monitoring Singlet/Triplet Interconversion in OLEDs — •Ulli von Goscinski, Dirk Hertel, and Klaus Meerholz — University of Cologne, Institute of Physical Chemistry, Luxemburger Str. 116, 50939 Cologne, Germany

In order to reach highest efficiencies in organic light-emitting diodes (OLEDs), excitons from both, singlet as well as triplet states, have to be harvested. Initially, they are distributed in a ratio of 1:3 according to spin statistics. Usually, a conversion between these states by intersystem crossing or reverse intersystem crossing is required to realize highly efficient OLEDs e.g. devices based on thermally activated delayed fluorescence (TADF) [1]-[2]. The rate of interconversion can be directly manipulated by small magnetic fields (< 150 mT). We utilize these magnetic field effects, namely magneto conductivity (MC), magneto electroluminescence (MEL) and magneto photoluminescence (MPL) to monitor singlet/triplet conversion events. The correlation of MEL and MPL is essential to clarify the underlying mechanism because of the different initial population of the singlet and triplet levels upon electro- or photoexcitation. Temperature dependent luminescence and conductivity measurements allow further insights in the nature of spin state conversion in organic emitter molecules.

[1] Zhang, Q. et al., *Nat. Photonics* 8, 326-332 (2014).

[2] Kaji, H. et al., *Nat. Commun.* 6, 8476 (2015).

CPP 37.26 Wed 11:00 Poster B1

Kinetic Monte Carlo simulations of energy transfer processes in an organic light emitting diode — •Leanne Paterson and Denis Andrienko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Organic light emitting diodes (OLEDs), utilise small organic molecules, in order to achieve an emissive electroluminescent layer. Ultra-thin, lightweight and flexible characteristics offer a highly enticing substitute, in comparison to their inorganic counterpart. It is therefore understandable why there has been a large amount of research, focused on enhancing the efficiency and stability of OLEDs. However, achieving a blue OLED, which is both efficient and stable, has proven to be problematic. The challenge originating with the limitations of the individual blue emitters, be that phosphorescent or fluorescent. Commercially, stability is prioritised, in order to achieve a long-lived consumer product, but with battery life on portable devices being the cost of any inefficiency, it is vital that blue OLEDs become more efficient. By developing a Kinetic Monte Carlo (KMC) code, for the study of excited molecule energy transfer, the individual emitters can be studied. Making direct comparisons to experimentally achieved results, it is possible to investigate processes, such as Förster resonance energy transfer (FRET) and Dexter energy transfer. Using the KMC code a unicoloured phosphor-sensitised fluorescence (UPSF) OLED and the corresponding energy transfer processes are explored. The fundamental efficiency and lifetime limits are identified, providing a clear insight, and expanding on experimentally achieved results.

CPP 37.27 Wed 11:00 Poster B1

Derivates of Imidazo[1,5-a]pyridine as Blue Light-Emitters for OLED — •Georg Albrecht[1], Carina Rössiger[2], Jasmin Martha Herr[2], Harald Locke[2], Hisao Yanagi[3], Richard Göttlich[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik — [2]Justus-Liebig-Universität Gießen, Institut für Organische Chemie — [3]Nara Institute of Science and Technology

1,3-disubstituted imidazo[1,5-a]pyridines are discussed for applications in material science as new and oxidation-stable blue emitters, e.g. for organic light emitting diodes (OLED). We investigated the stepwise change of physical properties in solution and solids when introducing nitrogen atoms and/or increasing sizes of aromatic rings as substitutional moieties. As an extension, a larger homologue, i. e., imidazo[1,5-a]quinoline was also studied. Absorption and emission spectra as well as quantum yields were measured and interpreted based on DFT calculations. Single crystals were grown from solution or by entrainer sublimation and thin films were prepared by physical vapor deposition. Fluorescence microscopy was used to investigate on crystal emission. Comparing the results obtained at thin films and in solution, the molecular coupling in the different phases is assessed and their applicability in OLED devices is discussed.

CPP 37.28 Wed 11:00 Poster B1

Excimer formation in carbazole-based host materials for OLEDs — •Eimantas Duda[1], Alexander Rudnick[1], Sergey Bagnich[1], Daniel Wagner[2], Peter Strohriegl[2,3], and Anna Köhler[1,3] — [1]Soft Matter Optoelectronics, Department of Physics, University of Bayreuth, Germany — [2]Macromolecular Chemistry I, Department of Chemistry, University of Bayreuth, Germany — [3]ayreuth Institute of Macromolecular Research, University of Bayreuth, Germany

We present a detailed spectroscopic study on bipolar OLED host materials in solution and in neat film from 10K to room temperature. The hole-transporting part is based on the carbazole moiety, while the electron-transporting part is based on triazine moiety. We find that the tendency to excimer formation depends sensitively on the planarity of the molecule, counterintuitively with more excimer formation for the planar ones. Quantum chemical calculations indicate that this results from excited state localization onto the outer carbazole moiety for the non-planar compounds.

CPP 37.29 Wed 11:00 Poster B1

Density of States at the Interface of Organic Permeable-Base Transistors — •Henning Iseke, Felix Dollinger, Hans Kleemann, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Dresden, Germany

Organic permeable-base transistors (OPBT) are among the best performing organic transistors reaching on/off ratios of $>10^8$ and transition frequencies of >40 MHz. These vertical transistors resemble solid-state triodes where the current is controlled by the potential of a permeable electrode denoted as base. As for other organic transistors, the knowledge of the interfacial density of states is a key in order to develop an in-depth understanding of the device operation as well as degradation processes. However, for OPBTs, this interfacial density of states has not been revealed so far.

D. V. Lang et. al proposed a method to determine the density of states in organic field effect transistors by means of temperature dependent transfer characteristics. Here, we validate this method and discuss under which conditions it is applicable to OPBTs. Furthermore, we carry out systematic device investigations under various stress conditions, and discuss how this stress affects the interfacial density of states. This study helps to develop a deeper understanding of the underlying mechanisms of degradation in OPBTs. Moreover, it enables more systematic approaches for device optimization due to the knowledge of the interfacial density of states.

CPP 37.30 Wed 11:00 Poster B1

Influence of Humidity on Work Function of PEDOT:PSS Thin Films — •Aman Anand[1,2], Rico Meitzner[1,2], Shahidul Alam[1,2], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Jena, Germany — [2]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Jena, Germany

Poly (3,4-ethylenedioxythiophene): poly (styrene sulfonate) (PEDOT: PSS) is the most common and successful commercial conductive polymer used in the field of optoelectronics. Its properties are high transparency in the visible range, high electrical conductivity, excellent chemical and physical stability, high ductility, good film-forming properties, and high work function among the other polymers. PEDOT: PSS is highly hygroscopic in nature, which limits its applications. In the present work, the influence of moisture content due to hygroscopicity of the PEDOT: PSS thin film is in regard to the change of work function. Different modifications on the PEDOT: PSS which wants to lead to better compatibility in forming contacts with organic semiconductors.

CPP 37.31 Wed 11:00 Poster B1

IR spectroscopic investigation of precursor aromatization of poly(p-phenylene) — •Rainer Bäuerle[1,2], Ali Abdulkarim[3], Karl-Philipp Strunk[1,4], Jan Freudenberg[2,3], Daniel Jänsch[2,3], Sebastian Beck[1,2], and Annemarie Pucci[1,2] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]InnovationLab, Heidelberg — [3]Organisch-chemisches Institut, Universität Heidelberg — [4]Centre for Advanced Materials, Universität Heidelberg

Two challenges of the long-desired prototype of a conjugated polymer semiconductor poly(para-phenylene) (PPP) are its difficult synthesis and its insolubility. Both problems have been recently overcome by a new precursor route. [1] We investigate and compare the thermal aromatization of a kinked and a linear precursor polymer using IR spectroscopy and UV-vis ellipsometry on thin films.

For a kinked precursor polymer we find that the aromatization speed increases with increasing temperature and decreases with decreasing layer thickness yielding unordered PPP induced by the unordered precursor.

In contrast to this, the aromatization kinematics of a linear precursor is independent from layer thickness and already the thin film of the precursor exhibits near-range order which is passed through to the converted PPP. The low conversion temperature (<250 °C) makes our PPP feasible for fabrication of plastic devices. It was further proven that PPP is long-time stable and shows no degradation.

[1] A. Abdulkarim et al., J. Am. Chem. Soc., 2016, 138 (50), pp 16208-16211

CPP 37.32 Wed 11:00 Poster B1

Polarisation anisotropy in organic guest-host systems — •Felix Höhnle, Thomas Morgenstern, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Exciting dye molecules with linearly polarised light leads to an anisotropic excited state population of the emitters' transition dipole moments (TDMs). Depending on different depolarisation effects before light emission –such as rotational diffusion (mostly in solutions), intra- and intermolecular exciton migration or conformational changes of molecules– the emitted light can also be partly polarised. The extent of the latter is quantified by the anisotropy value r. It relates the intensities emitted with polarisation parallel and perpendicular with respect to the polarisation of the exciting light.

In this work we probed thin solid films of commonly used organic emitters doped into a matrix. It could be shown that polarisation anisotropy can be increased by decreasing the dye concentration in the guest-host system, which must be due to reduced intermolecular exciton transfer since no other processes should be present in a solid film. Depending on the exact material, values close to the theoretical maximum of $r = 0.4$ were reached. Additionally, we see that excess energy of excitons affects the migration process and thus the anisotropy.

The above effect can also influence TDM orientation measurements which aim to improve device efficiencies. At low dye concentrations, the hindered equilibration of excitons to all orientations upon light emission can lead to erroneous (pseudo-horizontal) orientation values.

CPP 37.33 Wed 11:00 Poster B1

Comparison of a solution-based doping process and doping via coevaporation for thin layers of organic semiconductors — •Marius Gebhardt, Theresa Linderl, Eduard Meister, and Wolfgang Brütting — Institute of Physics, University of Augsburg, Germany

For the use of organic layers in thermoelectric devices a high electrical conductivity and Seebeck coefficient combined with low thermal conductivity is essential. In this work we focus on increasing the electrical conductivity by different doping approaches.

Thin evaporated layers of the electron donor molecules DIP, 6T and DBTTF, on top of which the strong electron acceptor F4-TCNQ dissolved in solution was spincoated, are compared to coevaporated layers with F6-TCNNQ as the electron acceptor. To study the degree of doping as well as to discern between ion pair (IPA) and charge transfer complex (CTX) formation the transmission spectra of the samples were measured. The impact of the doping processes on the surface and bulk morphology was examined via atomic force microscopy and X-ray diffraction. Strong indications for the formation of charge transfer crystals are observed in some of the discussed material combinations. First conductivity measurements, however, indicate that the electrical transport is affected in different ways.

CPP 37.34 Wed 11:00 Poster B1

From spin-coating to slot-die printing in organic solar cells: Where do we lose the efficiency? — •Daniel Kroh[1], Jegadesan Subbiah[2], Doojin Vak[3], David Jones[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth — [2]School of Chemistry, Bio21 Institute, University of Melbourne, Australia — [3]CSIRO Manufacturing, Melbourne, VIC 3168, Australia

The field of solution-processed organic solar cells (OSCs) has been dominated by polymeric semiconductors, though molecular materials with high power conversion efficiencies (PCEs) in OSCs have been reported and are attractive due to their reduced batch-to-batch variation. For example, devices based on the donor molecule BQR are thermally stable and show a low thickness dependence of the active layer with PCEs reaching 10.7%. These properties suggest BQR as an excellent choice for roll-to-roll processing, which is relevant for industrial fabrication. However, within the transition from spin coated to slot-die printed devices a drop in efficiency appears. Although this drop is commonly observed, its reason is not clear. We use time resolved and temperature dependent UV-Vis absorption and photoluminescence spectroscopy to investigate the formation of spin-cast and slot-die coated films and the resulting morphology in-situ during the deposition process of BQR:PC70BM blends. Comparing the two deposition methods allows us to get a better understanding of the correlation between film morphology and device performance. With this insight, we can optimize the conditions of the slot-die printing process to reduce the drop in PCE, which is an important step towards industrial fabrication.

CPP 37.35 Wed 11:00 Poster B1

Understanding the mechanism behind the novel doping of organic semiconductors via Lewis Acids — •Simon Biberger[1], Viktor Brus[2], David Cao[2], Brett Yurash[2], Dirk Leifert[3], Thuc-Quyen Nguyen[2], and Anna Köhler[1] — [1]Experimental Physics II, University of Bayreuth, Bayreuth, Germany — [2]Center for Polymers and Organic Solids, UCSB, Santa Barbara, USA — [3]Organisch-Chemisches Institut, Westfälische Westfälische Wilhelms-Universität, Münster, Germany

To p-dope organic semiconductors F4TCNQ is commonly used. This doping mechanism relies on the electron transfer from the HOMO of the semiconductor to the LUMO of the dopant. This occurs by a match of those energy levels. For a solution-processed semiconductor this approach suffers from the differential solubility of the dopant, the charge-transfer complex and of the polymer what ultimately limits the processability of the doped semiconductor. In this study we use electrophilic Lewis acids to p-dope conjugated polymers. Work by Zalar et al. (Adv. Mat. 2014, 26, 727-727) showed an increased mobility after addition of Lewis acid. Yet the mechanism behind this doping approach is still elusive. To understand this approach we systematically investigate the effect of structural and electronic factors by varying, e.g., the donor and acceptor strength of the polymer. Optical and electrical characterization, using, e.g., optical spectroscopy and EPR, were performed to understand the influence of the adduct formation on the properties of the polymer.

CPP 37.36 Wed 11:00 Poster B1

Consequences of Ionic Adsorption on the Photovoltage in Dye-sensitized Solar Cells — •Raffael Ruess[1], Sabina Scarabino[2], Andreas Ringleb[1], Kazuteru Nonomura[3], Nikolaos Vlachopoulos[3], Anders Hagfeldt[3], Gunther Wittstock[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik — [2]Universität Oldenburg, Institute of Chemistry — [3]Ecole Polytechnique Federale de Lausanne, Institute of Chemical Sciences and Engineering

Reversible redox couples that allow faster charge transfer than the classical I^-/I_3^- can improve the performance of dye-sensitized solar cells (DSSCs). In our work we study a cationic Co-based redox couple that promises high open-circuit photovoltages V_{oc} by reducing the energy-loss during the dye regeneration process. However, we found that such cations lead to different surface reactions with oxide semiconductors compared to the anionic I^-/I_3^-. By using photoelectrochemical and optical techniques we noticed that the semiconductor surface charge plays a major role in determining V_{oc} by stabilizing or destabilizing the electronic states in the semiconductor. Further, light-harvesting of the dye is influenced by electric fields arising from adsorbed ions at the semiconductor surface inducing a Stark effect on the molecular orbitals. We conclude that the ionic character of electrolyte components such as the redox couple or electrolyte additives significantly influence the energetics in the cell and, thus, V_{oc}. Our work shows that the control of semiconductor surface charge is key in improving the DSSC performance.

CPP 37.37 Wed 11:00 Poster B1

Comparison of sequential and solution-mixed doping of poly(3-hexylthiophene) in thin films using the Lewis acid BCF — •Dominique Lungwitz[1], Ahmed E. Mansour[1], Andreas Opitz[1], and Norbert Koch[1,2] — [1]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

Molecular doping of organic semiconductors is a commonly used technique to increase the conductivity and tune the electronic structure. Sequential doping method allows for an improved film morphology with controlled dopant load by avoiding agglomeration of polymer and dopant before deposition as observed partially for solution-mixed doping [1]. Herein, we investigate the changes in the electronic structure by photoemission spectroscopy and dopant distribution for sequentially and solution-mixed doping of poly(3-hexylthiophene) (P3HT) in regiorandom (RRa) and regioregular (RRe) forms. The Lewis acid dopant tris(pentafluorophenyl)borane (BCF) is applied for p-doping. We find that the solution-mixed process results in homogeneous bulk doping with an increase in the ionization energy for both P3HT regularities. However, for sequential doping by vapour exposure of thin RRa-P3HT films, a saturation for the BCF load is found at the surface and Fermi-level pinning is observed due to interfacial doping of the top polymer surface. Furthermore our results demonstrate that dopant molecules tend to diffuse more in RRe-P3HT than in RRa-P3HT films once they are sequentially doped and result in intermixed doped P3HT similar to solution mixed doping.

CPP 37.38 Wed 11:00 Poster B1

Thiophene based Semiconductors and Graphene Oxide for Organic Solar Cells — •Roy Schaffrinna[1,2], Martina Schwager[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Hochschule München, Fakultät für Angewandte Naturwissenschaften und Mechatronik, 80335 München

The polymers poly(3-hexylthiophene), poly(3-thiopheneacetic acid), poly(3-thiopheneethanol) and the related copolymers are prepared starting from the respective monomer units by chemical oxidative polymerization. Graphene has also been oxidized to graphene oxide, which due to its functional groups is much more soluble in organic solvents and forms far more homogeneous layers than pure graphene and is also liquid processable. The synthesized molecules are used either as electron donor or electron acceptor in the organic solar cell and are characterized via infrared, absorption and fluorescence spectroscopy.

The organic materials are electrically conductive due to their extended conjugated π-electron system and therefore require neither heavy metals / heavy metal complexes nor dopants for charge transport and can be easily deposited via spin-coating from a solution.

CPP 37.39 Wed 11:00 Poster B1

Molecular orientation of diketopyrrolopyrrole (DPP)-based donor-acceptor copolymers in thin films — Andreas Früh[1], •Sven Bölke[1], Florian Trilling[2], Ullrich Scherf[2], Thomas Chassé[1], and Heiko Peisert[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tuebingen, Auf der Morgenstelle 18, 72076 Tuebingen, Germany — [2]Makromolekulare Chemie und Institut für Polymertechnologie, Bergische Universität Wuppertal, Gaussstrasse 20, 42119 Wuppertal, Germany

Novel low band gap (LBG) polymers are interesting materials for organic-based devices because of their high absorption in the solar spectrum and favourable electronic properties. For applications, the self-organization in thin films is an important issue in which the chemical structure determines largely the arrangement of the polymer chains.

Promising materials in this context are diketopyrrolopyrrole(DPP)-based donor-acceptor copolymers, where the DPP unit is inscribed into a double-stranded ladder framework leading to partially ladderized step-ladder polymers with high charge transfer mobilities, attributed to the highly aggregated, π-stacked conformation of DPP.

In the present study, we use polarization dependent IR spectroscopy in transmission to investigate the preferred orientation of DPP-based donor-acceptor copolymers in about 300 nm thin films. Analyzing vibrations with differently oriented transition dipole moments, we discuss the preferred molecular orientation of the polymers in context with the chemical structure. Transition dipole moments were calculated using DFT.

CPP 37.40 Wed 11:00 Poster B1

Following the morphology formation of printed non-fullerene active layer for solar cells — •Xinyu Jiang[1], Sebastian Grott[1], Tommaso Riccitelli[1], Volker Körstgens[1], Kerstin Wienhold[1], Matthias Schwartzkopf[2], Stephan V. Roth[3], Wei Cao[1], Shanshan Yin[1], Lin Song[1], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]DESY, Notkestr. 85, 22607 Hamburg — [3]KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden

Bulk heterojunction (BHJ) organic solar cells have gained significant improvements via novel organic synthesis methods and optimized fabrication routes, especially with respect to their potential roll-to-roll processing for large-area device manufacturing. Printing techniques allow for up-scaling to industrial-oriented scale which is not the case for laboratory deposition techniques like spin coating. In the present work, we fabricated an active layer which contains a low band gap donor polymer(pffBT4T-2DT) with a non-fullerene acceptor(EH-IDTBR) for solar cells by using a slot-die printing technique. To observe the structure formation of polymer domains at a larger length scale, grazing incidence small-angle X-ray scattering (GISAXS) was used in-situ during the printing process. BHJ solar cells based on printed active layer film were fabricated, which showcases the suitability of the printing technique.

CPP 37.41 Wed 11:00 Poster B1

Investigation on the influence of morphological modifications on the power-conversion efficiency of fullerene-free organic solar cells — •Goran Ivkovic Ivandekic, Sebastian Grott, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Highly efficient organic solar cells have received significant attention in recent years. The properties, such as light weight, flexibility and the possibility to be processed at low cost, allow a wide range of application in the field of electronic devices. Although great progress has been made with fullerene-based cells, weak light absorption in the visible spectrum along with high production costs of fullerene derivatives is motivating the increased effort in developing a promising alternative. This study attempts to further improve fullerene-free organics solar cells by modifying the morphology of the photo-active layer. To substitute the fullerene, ITIC is chosen, and a low-bandgap PBDB-T is used. Different PBDB-T:ITIC bulk-heterojunction blends are processed by varying the solvents. The prepared solar cells are characterized using several experimental techniques. To get insight into the inner morphology of the applied bulk-heterojunction grazing-incidence small-angle X-ray scattering (GISAXS) and grazing-incidence wide-angle X-ray scattering (GIWAXS) are used. These information are related to photo-electronic characteristics obtained from UV-vis and PL measurements and current density-voltage curves, in order to get a full understanding of the applied donor-acceptor system.

CPP 37.42 Wed 11:00 Poster B1

Photophysical properties of ternary non-fullerene organic solar cells — •Ali Sahin, Dirk Hertel, and Klaus Meerholz — University of Cologne, Luxemburgerstr.116, Cologne, Germany

Organic solar cells (OSC) are considered an attractive alternative to conventional inorganic solar cells. The benefits OSC offer, result from their favorable low-cost fabrication and their application in thin-film form. The active layer of an OSC is typically composed of two components in a bulk-hetero junction (BHJ) mixture, an electron donor (p-type semiconductor) and an electron acceptor (n-type semiconductor). Upon light excitation the formed exciton has to diffuse by typically 10-30nm to reach to D-A interface, where it dissociates into free charge carriers. Fullerene derivatives have dominated as acceptors for many years, but recently non-fullerene acceptors - mostly of ADA motif - have entered the scene [2]. Ternary BHJ cells with three components in the active layer represent one way to finetune the interface. Therefore, a series of new n-type ADA-acceptors were investigated with regard to their photophysical properties and in combination with various p-type conjugated polymers. Conductivity measurements of the neat materials and mixtures were carried out in field-effect transistors and compared with the photo-CELIV and TPV measurements in corresponding BHJ films. The charge carrier lifetime and the recombination rates were determined in order to correlate the molecular properties and BHJ properties in the thin-film with the photovoltaic parameters in binary and ternary OSC.

[2] Y. Lin et al., J. Am. Chem. Soc., 2016, 138(9), 2973-2976.

CPP 37.43 Wed 11:00 Poster B1

N-type C_{60} thin films for thermoelectric applications — •Konstantin Barko[1], Alexander Steeger[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Efficient waste heat recovery by thermoelectric generators requires p- and n-type semiconductors with high figures of merit $zT{=}\sigma S^2T/\kappa$. Therefore, it is a key challenge to find materials with a high ratio of electrical conductivity σ to thermal conductivity κ. In this regard, organic semiconductors appear an appropriate class of compounds as they offer low thermal conductivities and can be doped to increase their electric conductivities. However, the search for stable n-dopants turns out to be challenging. As a promising host, fullerene C_{60} thin films has shown κ-values as low as 0.16 W/(mK)[1] and have been successfully n-doped with acridine orange base [2]. Using this material combination as a starting point, we analyze the thermoelectric characteristics of n-doped C_{60} thin films as function of dopant concentration in the relevant temperature range from 300 K to 400 K. The transport properties are discussed in relation to the underlying thin film morphology estimated by AFM and X-ray diffraction. Furthermore, we pursue the concept of tuning the relative positions of transport-level and Fermi-energy which determines the macroscopic Seebeck coefficient S. These results are discussed in view of implementing n-doped fullerene layers in thin film thermoelectric generators. [1] M. Sumino et al. Appl. Phys. Lett. 99(2011)093308 [2] F. Li et al. J. Appl. Phys. 100(2006)023716

CPP 37.44 Wed 11:00 Poster B1

Investigating Triplet Exciton Losses in PBDB-T:ITIC Bulk Heterojunction Solar Cells — •Johannes Junker[1], Maria Kotova[1], Alberto Privitera[2], Andreas Sperlich[1], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Department of Physics, Oxford University, Oxford, United Kingdom

Organic bulk heterojunction solar cells based on small molecule non-fullerene acceptors (NFA) received a lot of attention in the past few years as their power conversion efficiency rapidly exceeded the 13% mark. So far, little is known about the photophysics of Polymer:NFA blends. By using spin-sensitive techniques, i.e. photoluminescence and electrically detected magnetic resonance (PLDMR, EDMR), we investigated triplet exciton generation in films of neat Poly[(2,6-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)-benzo[1,2-b:4,5-b']dithiophene))-alt-(5,5-(1',3'-di-2-thienyl-5',7'-bis(2-

ethylhexyl)benzo[1',2'-c:4',5'-c']dithiophene-4,8-dione)] (PBDB-T), 3,9-bis(2-methylene-(3-(1,1-dicyanomethylene)-indanone))-5,5,11,11-tetrakis(4-hexylphenyl)-dithieno[2,3-d:2',3'-d']-s-indaceno[1,2-b:5,6-b']dithiophene (ITIC), their blends and solar cells. In all films we found triplet excitons and CT states at low temperatures. However, in devices operated at ambient conditions, the triplets disappear. We discuss these results in a picture of strongly suppressed triplet exciton generation compared to fullerene-based solar cells.

CPP 37.45 Wed 11:00 Poster B1

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]Soft matter optoelectronics, 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 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). However, computational models to investigate this morphology-mobility relationship are still rare. Here, we have developed a kinetic Monte Carlo model approach to simulate charge transport in OFETs that greatly reduces the computational costs at higher charge-carrier concentrations through an effective energy landscape. This is necessary in order to simulate larger device sizes enabling the introduction of morphological aspects. Our model enables us to study the influence of conjugation length and their alignment in the film in the charge transport process.

CPP 37.46 Wed 11:00 Poster B1

Dipolar doping of organic semiconductors to enhance carrier injection — •Alexander Hofmann[1], Vivien Wessels[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

We have investigated the prototypical polar organic system *N*,*N*'-Di(1-naphthyl)-*N*,*N*'-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB) doped with tris-(8-hydroxyquinolate) aluminum (Alq_3) in different ratios by various electrical and optical techniques. Throughout all devices and measurements, a maximum of injected charge carriers and current for low to moderate doping ratios is observed. The strong dipole moment of polar organic materials like Alq_3, if not oriented perfectly isotropic, will lead to the buildup of a giant surface potential (GSP). It has been shown previously, that depending on polarity and carrier species, injection can be improved or hindered[1]. By combining electrical[2] and optical measurements as well as simulations, we find a complex relation of positive and negative effects on overall device performance that, besides the influence of the GSP on injection and doping on transport, also reveal a change in NPB energy levels provoked by the dipolar surrounding.

[1] Organic Electronics **39**, 244-249 (2016) [2] Journal of Applied Physics **122**, 115502 (2017)

CPP 37.47 Wed 11:00 Poster B1

Charge transfer effects in donor and acceptor mixed systems of DNTT and PDIF-CN$_2$ — •Nadine Russegger, Lena Merten, Alexander Hinderhofer, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Germany

One very important and fundamental process for organic semiconductors (OSCs) is the charge transfer effect between electron donor and electron acceptor molecules.

In this work, the charge transfer effect of weakly interacting organic semiconductor thin film mixtures is comprehensively investigated. We choose dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene (DNTT) as donor and N,N'-1H,1H-perfluorobutly-dicyanoperylene-3,4:9,10-bis(dicarboxyimide) (PDIF-CN$_2$) as acceptor.

The structural, optical and electronic properties of the intermolecular interactions were characterized using a range of experimental methods. The structure of the mixed phase polymorph was evaluated by surface X-ray scattering. The charge transfer in the equimolar mixed film of DNTT and PDIF-CN$_2$ was characterized by absorption, photoluminescence as well as in-situ differential reflectance spectroscopy.

The results allow us to determine correlations between structural properties and charge transfer effects within the mixed systems of DNTT and PDIF-CN$_2$.

CPP 37.48 Wed 11:00 Poster B1

Mixing behaviour of small molecule organic semiconductors 6T and PDIF-CN$_2$ — •Lena Merten, Nadine Russegger, Alexander Hinderhofer, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Germany

Mixtures of small molecule organic semiconductors are a promising research field due to their various applications in organic electronics. For most applications a specific degree of order and mixing is desired, thus the mixing behaviour of dissimilar organic molecules is to be investigated.

We prepared thin films from mixtures of α-sexithiophene (6T) and N,N'-1H,1H-perfluorobutyl-dicyanoperylene-3,4:9,10-bis(dicarboxyimide) (PDIF-CN$_2$), as donor and acceptor type molecules, respectively.

The mixed films exhibit strong long-range phase separation. Film properties were characterized structurally and optically during and after growth. The structural characterizations were done post-growth by AFM and X-ray scattering, the optical investigation by absorption spectroscopy, photoluminescence and ellipsometry, complemented by in-situ differential reflectance spectroscopy to monitor the evolution of optical properties during growth.

CPP 37.49 Wed 11:00 Poster B1

Morphology Formation and Stability of Organic Supramolecular Structures — •Asena Cerhan[1], Christopher Greve[1], Michael Buchhorn[1], Bernd Wittmann[2], Felix Wenzel[3], Hans-Werner Schmidt[3], Richard Hildner[2,4], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung-Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth — [2]Lehrstuhl für Spektroskopie weicher Materie, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth — [3]Makromolekulare Chemie I, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth — [4]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4 9747 AG Groningen, Netherlands

Organic, supramolecular systems can exhibit extreme transport properties. To understand such fascinating material properties, we study the morphology of such systems under various external conditions. As the aromatic interactions have great effects on the temperature-dependent dynamic behaviour of supramolecular assemblies, the temperature studies were combined with scattering experiments. Using chemically different material systems and studying their structure in various solvents in solution, but also in thin films, we systematically investigate the importance of chemical composition versus processing conditions on the final self-assembled (super-)structure. The temperature studies with simultaneous scattering and photoluminescence measurements, furthermore, lend us insights into the stability and formation of such organic, supramolecular structures.

CPP 37.50 Wed 11:00 Poster B1

influence of UV-light on charge injection across hybrid metal oxide/organic interfaces — •Meysam Raoufi, Ulrich Hörmann, and Dieter Neher — Institute of Physics and Astronomy, University of Potsdam, Potsdam

Selective charge injection into organic semiconductors is crucial for the performance of organic opto-electronic devices. Surface modification of metal oxides with self-assembled monolayers (SAMs) allows engineering of the work function (WF) to align with the charge transport levels of organic semiconductors. [1] At the same time, it has also been shown that irradiation with UV-light (light-soaking) has a pronounced effect on the electronic properties of metal oxides [2]. Here, we study the combined effect of light-soaking and surface modification on the WF and hole injection properties of ZnO. By Kelvin probe measurements in a UV-free environment we determine the WF of SAM modified ZnO prior to and after intentional light-soaking. We carefully modulate the level of photo-doping of the metal oxide layer and track the WF changes. This allows us to correlate the hole injection current from ZnO into P3HT in unipolar devices with the change in injection barrier height. Our results illustrate a severe dependence of the ZnO/organic contact on the history of light exposure. Valid conclusions about the contact energetics are only possible, if the sample history is precisely known. Importantly, despite being considered as a typical n-type material, properly treated ZnO forms an ohmic contact for hole injection.[1] I. Lange et al., Appl. Phys. Lett. 106, (2015). [2] G. Lakhwani et al., J. Phys Chem C. 114, (2010).

CPP 37.51 Wed 11:00 Poster B1

Long-term durability measurement of LHC-based DSSC under constant illumination — •Aike Weissmann[1], Fabian Schmid-Michels[1], Nina Lämmermann[2], Lutz Wobbe[2], Andreas Hütten[1], and Olaf Kruse[2] — [1]Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany — [2]Faculty of Biology, Algae Biotechnology & Bioenergy, Bielefeld University, Germany

With the recent surge in interest in ligh harvesting complexes (LHC) as a substitution for more traditional choices of dye in dye-sensitized solar cells (DSSC), the question of stability of the biological compounds becomes more pressing. LHC are required to withstand effects of photobleaching, heat and possibly hostile electrolytic environments to ensure the longevity of the created devices. This is necessary for LHC to be able to become a low-cost, low-toxicity alternative to the more commonplace dyes. To this end, LHC-based DSSC have been kept under constant illumination for an extended ($>$ 48h) period of time, while their power output, short-circuit current and open-circtuit voltage had been measured at least once per hour.

CPP 37.52 Wed 11:00 Poster B1

Investigation of Sub-Molecular Parts in Mixtures for Organic Photovoltaics — •Arthur Markus Anton[1], Rico Meitzner[2], Shahidul Alam[2], Harald Hoppe[2], and Friedrich Kremer[1] — [1]Peter Debye Institute for Soft Matter Physics, Leipzig University — [2]Center for Energy and Environmental Chemistry Jena, Friedrich Schiller University Jena

Nowadays, renewable sources of energy together with low-cost device manufacturing are highly demanded. For this purpose, the application of organic photovoltaics (OPV) appears to be suitable for reducing environmental impact as well as direct technology cost by "green" and low-cost synthesis combined with great-scale casting methods. Despite the advantages of fullerenes in OPV, such as high electron mobility or a low LUMO energy level, their commercial application is restricted through high synthesize costs and chemical instabilities. In order to overcome these detriments, non-fullerene acceptors have obtained considerable attention. Blends of PBDB-T:ITIC achieved efficiencies up to 11% in bulk heterojunction solar cells [1]; blends of AnE-PVstat:ITIC, instead, fall short, although photoluminescence indicates efficient quenching of donor emission [2]. It is believed that orientation and order of molecular units play an essential role for the performance of organic semiconductors [3]. Thus, a novel approach by means of FTIR spectroscopy is employed in order to analyze submolecular parts in polymer:acceptor bends. [1] W. Zhao et. al., *Adv. Mater.* **28** (2016), 4734; [2] S. Alam et. al., *Chem. Pap.* **72** (2018), 1769; [3] A. M. Anton et. al., *J. Am. CHem. Soc.* **137** (2015)

CPP 37.53 Wed 11:00 Poster B1

Determination of morphological evolution in bulk heterojunction polymer solar cells — •Hongwon Kim, Tommaso Riccitelli, Xinyu Jiang, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Organic solar cells have been progressed via novel organic materials indicating improved efficiencies as well as high stability. Bulk heterojunction (BHJ) polymer solar cells offer the advantage of a high power/mass ratio combined with a mechanical flexibility. However, the achieved best efficiency values still stay behind that of other solar cell technologies, which demonstrates the needs for more fundamental understanding. In the present study, BHJ solar cells are investigated which consist of a low-bandgap donor (PffBT4T-2OD) and a non-fullerene acceptor (EH-IDTBR). The active layers are investigated with X-ray scattering techniques to track morphological evolution during the ageing processes via different external conditions. In addition, with spectroscopic measurements under identical conditions we get insights into changes on a molecular level.

CPP 37.54 Wed 11:00 Poster B1

Coupled organic-inorganic nanostructures with mixed linker molecules — •Florian Grassl[1], Eduard Meister[1], Andre Maier[2], Marcus Scheele[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Institute for Physical and Theoretical Chemistry, University of Tübingen, 72076 Tübingen, Germany

Coupled organic-inorganic nanostructures (COINs) utilize organic semiconductors as crosslinking ligands to facilitate charge conduction between semiconductor nanocrystals. They offer the perspective to combine efficient carrier transport with a high degree of structural order [1], as it has been successfully demonstrated in field-effect transistors [2]. A well-known and working organic ligand is 1,2-Ethanedithiol (EDT), especially with PbSe nanocrystal [3]. Here we focus on the introduction of a mixture of two organic ligands. Using the dip-coating technique of fabricating COIN layers from PbS nanocrystal with a mixture of Zinc β-Tetraaminophthalocyanine (Zn4APc) and EDT as organic linker molecules, we elucidate the carrier transport and device performance. We compare this mixture of linker molecules with single Zn4APc- and EDT-ligands in transistors, diodes and solar cells.

[1] M.Scheele *et.al.*, Physical Chemistry Chemical Physics (2015), doi:10.1039/c4cp03094j

[2] A.André *et al.*, Chemistry of Materials (2015), doi:10.1021/acs.chem mater.5b03821

[3] J.Luther *et al.*, Nano Letters (2008), doi:10.1021/nl802476m

CPP 37.55 Wed 11:00 Poster B1

Investigation of the templating effect of graphene on organic molecular layers — •Max Reimer, Selina Olthof, and Klaus Meerholz — University of Cologne, Luxemburger Str. 116, Germany

Electrical and optical properties of many organic semiconducting molecules are highly anisotropic. Therefore these properties will depend on the packing and ordering motif when deposited as thin films. However, most of the time when such molecules are used in organic electronic devices the growth mode is rather amorphous. Being able to grow layers with an engineered order could dramatically improve their properties such as absorption, emission, and most importantly mobility [1]. In the past years, monolayer graphene has proven to be a useful templating material [2] for subsequent material growth. Using this approach and optimizing the preparation conditions we are able to achieve an ordered and oriented growth mode for merocyanine dyes; this versatile material class is highly interesting for the use in organic photovoltaics. Two in-situ methods, low energy electron diffraction (LEED) and ultraviolet photoelectron spectroscopy (UPS), allow us to observe the packing motif and the width of the energetic levels in the region of the highest occupied molecular orbital (HOMO) which is connected to the degree of order of the molecular layer. We further exploit atomic force microscopy (AFM) which provides information about the grain size of the formed crystalline regions. The optimized film growth allows us to improve the IV characteristic of basic organic devices containing these molecules. [1] Guillaume Schweicher et al., IJC 2014, 54, 595-620 [2] Ti Wang et al., Sci. Rep. 2016, 6, 28895

CPP 38: Polymer Networks and Elastomers

Time: Wednesday 11:30–12:45 Location: H18

CPP 38.1 Wed 11:30 H18

Simulation and theory of model sliding-ring polymer systems — •Toni Müller[1,2], Michael Lang[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymer- forschung Dresden — [2]Technische Universität Dresden

In order to understand the elasticity of polymers which are harnessed by slidable rings such as polyrotaxanes we consider a simple model system. Here two chains are connected by crosslinking two of the slidable rings which act as stoppers for the other rings threaded on the chains. For the case of ideal chain statistics the partition function for chains under constant force can be calculated exactly and the resulting force-extension relations are compared with Monte Carlo simulations using the bond fluctuation model. We observe a strong strain-softening of the double-chain system under force which sharpens towards a jump-like transition of the elastic modulus for longer chains. We show that the reason for this behavior is fact that the slidable rings form a 1D real gas which is compressed by the stoppers if the chains are extended. Only if the external force exceeds the internal pressure caused by the slidable rings the chains can respond with the elastic compliance of their full contour related with a jump-like decay in modulus. Using simple thermodynamic arguments we calculate the critical force, and from an analytic approximation of the partition function we obtain the modulus of the connected chains in the low force region. Our system provides insights into a new class of elastic matter where conformational and internal degrees of freedom act together. A possible extension of our model are 'sliding-ring' gels build-up from many sliding-ring polymers.

CPP 38.2 Wed 11:45 H18

Microphase separation in cross-linked copolymers — •Gaoyuan Wang, Annette Zippelius, and Marcus Müller — Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen, Deutschland

Using particle-based simulations of a soft, coarse-grained model in conjunction with the Single-Chain-in-Mean-Field algorithm we have studied the cross-linking of (diblock) polymer melts and the subsequent microphase separation the cross-linked systems upon increasing the incompatibility, χN, between the two blocks. Without cross-linking, the simulated order-disorder transition (ODT) between a lamellar and a disordered liquid is shifted away from the mean-field prediction χN = 10.5 and is of first-order. With increasing cross-link density, the χN, at which the ODT occurs (for fixed cross-link density), shifts to larger values. Beyond the cross-link density of 1 per chain a gradual formation of a microemulsion-like structure (disordered gel) is formed, i.e., the morphology features a characteristic length scale but not long-range order. When we cross-link a lamellar liquid at χN > χODT and decrease χN, the χN at which the ODT occurs (i.e. long-range order is lost) differs from the previous one.

CPP 38.3 Wed 12:00 H18

Reversible magnetomechanical collapse in a soft elastic matrix — Mate Puljiz[1], Shilin Huang[2], Karl A. Kalina[3], Johannes Nowak[3], Stefan Odenbach[3], Markus Kästner[3], Günter K. Auernhammer[2], and •Andreas M. Menzel[1] — [1]Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany — [2]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [3]Technische Universität Dresden, Dresden, Germany

Embedding rigid particles in an elastic matrix hinders their motion. Under mutual attraction, their displacement leads to elastic deformations of the elastic environment. Counteracting restoring forces result.

Nevertheless, as we demonstrate, a reversible particle approach up to virtual touching is possible. For this purpose, the behavior of magnetizable nickel particles in a soft elastic gel matrix was analyzed in experiments [1]. Switching on and off an external magnetic field, the particles reversibly collapse towards each other and subsequently reseparate. Explicit analytical calculations and finite-element simulations describe and quantify these experimental observations [1].

The effect should be interesting from an application point of view. In magnetorheological elastomers, the overall material stiffness can be reversibly tuned by external magnetic fields acting on embedded magnetizable particles [2]. Induced formation of chain-like aggregates is possible. An associated material stiffening could be maximized by induced virtual touching of the embedded particles.

[1] M. Puljiz et al., *Soft Matter* **14**, 6809 (2018).
[2] G. Pessot et al., *J. Phys.: Condens. Matter* **30**, 125101 (2018).

CPP 38.4 Wed 12:15 H18

FORCs diagrams for magnetoactive elastomers studying by molecular dynamics simulations — •Alla Dobroserdova[1], Pedro Antonio Sanchez Romero[1,2], 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 FORCs (first-order reversal curves) diagrams to study how the matrix influences internal magnetic interactions. We consider several models of magnetoactive elastomers. We use the Molecular Dynamics Simulations to study the different systems. In order to introduce the elastic interactions we consider fixed nonmagnetic particles which are connected with dipolar ones by springs. As the simplest case, we consider spherical magnetic particles in an elastic matrix. As an extension, we take into account the shape anisotropy of magnetic particles. We also study magnetic particles with flake-like shapes. In order to plot the FORCs distribution we use a classical method [C. R. Pike et al., J. Appl. Phys. 85, 6660 (1999)]. 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 38.5 Wed 12:30 H18

Magneto-active elastomeric (MAE) films and their properties — •Sofia Kantorovich[1,2], Elena Minina[1,2], Elena Kramarenko[3], and Pedro Sánchez[1,2] — [1]University of Vienna — [2]Ural Federal University — [3]Moscow State University

Due to advances in synthesis, it is nowadays possible to prepare thin layers of elastomers with relatively high loading of magnetic particles. Such layers show a dramatic change of the hydrophobicity when an external magnetic field is applied. This effect is a consequence of the conventional chain formation of magnetic particles aligned along the magnetic field that causes not only the matrix deformation of the layer, but also roughens its surface. We study structural, magnetic and mechanical properties of such MAE layers by means of MD computer simulations. We develop a model of a MAE layers that captures the dependence of its surface roughness on the elastic properties of the polymer matrix and the magnetic interactions [1]. To examine elastic properties of these layers we consider them under action of an external magnetic field of different strength. We observe that the magnetic field stiffens the layer making it more robust to deformations. [1] P.Sanchez et al, Soft Matter 2018.

CPP 39: Focus: Controlling Phase Formation Dynamics in Solution Processed Semiconductors - organized by Christoph Brabec, Jens Harting and Hans-Joachim Egelhaaf

Time: Wednesday 15:00–18:45 Location: H14

Invited Talk CPP 39.1 Wed 15:00 H14

Film formation, microstructure and ferroelectricity of MAPbI3 light-harvesting layers — Holger Röhm[1,2], Tobias Leonhard[1,2], Alexander Schulz[1,2], Susanne Wagner[1,3], Michael Hoffmann[1,3], and •Alexander Colsmann[1,2] — [1]Karlsruhe Institute of Technology (KIT), Material Research Center for Energy Systems, Strasse am Forum 7, 76131 Karlsruhe, Germany — [2]Karlsruhe Institute of Technology (KIT), Light Technology Institute (LTI), Engesserstrasse 13, 76131 Karlsruhe, Germany — [3]Karlsruhe Institute of Technology (KIT), Institute for Applied Materials - Ceramic Materials and Technologies (IAM), Haid-und-Neu-Strasse 7, 76131 Karlsruhe, Germany

Among the remarkable properties of MAPbI3 is its ferroelectricity. Since the ferroelectric polarization influences the charge carrier recombination and transport, the orientation and shape of polarized domains within grains directly influences the device performance. This renders engineering of the grain orientation and size pivotal for the optimization of perovskite solar cells. In a combined EBSD, PFM and KPFM study, we spatially resolve and correlate the crystal orientation and the ferroelectric polarization of MAPbI3 with sub-grain resolution. These tools are indispensable for the relation of the microscopic thin-film structure to the optoelectronic device properties as they allow to monitor film formation, device optimization and to understand fundamental processes in perovskite solar cells. Understanding the microstructure and the film formation will not least be the key to future ab-initio engineering of new non-toxic and efficient solar cells.

Invited Talk CPP 39.2 Wed 15:30 H14

How do evaporating thin films evolve? Unravelling phase-separation mechanisms during solvent-based fabrication of polymer blends — •Olga Wodo — University at Buffalo, Materials Design and Innovation Department

Solvent-based fabrication is a flexible and affordable approach to manufacture organic thin films made from any combination of polymer, copolymers and/or small molecules. It is of paramount importance to understand morphology evolution during fabrication. However, it is challenging to experimentally visualize morphology evolution during processing.

In this talk, I will present our computational model to predict the evolving three-dimensional morphology during the fabrication of organic thin films. I will focus on multiscale challenges that when addressed allowed to resolve nano-morphological features while being able to simulate device scale domains. More importantly, I will discuss four modes of phase formation and subsequent propagation within the thinning film during solvent-based fabrication. I will address fundamental questions such as when and where phases are formed, and how they evolve to form the final structure. Finally, I will demonstrate how this analysis can be leveraged to ask questions on manufacturing designs with the ultimate goal of precise, yet affordable, morphology manipulation for a large spectrum of applications.

CPP 39.3 Wed 16:00 H14

Supramolecular structures of amphiphilic dyes for photochemical and photophysical applications — •Martin Presselt[1,2,3], Maximilian Hupfer[1,2], Martin Kaufmann[1], Felix Herrmann-Westendorf[1,2], Saunak Das[1,2], and Benjamin Dietzek[1,2] — [1]Friedrich Schiller University Jena, Helmholtzweg 4, 07743 Jena, Germany — [2]Leibniz Institute of Photonic Technology (IPHT), Jena, Germany — [3]sciclus GmbH & Co. KG, Moritz-von-Rohr-Str. 1a, 07745 Jena, Germany

Beyond molecular properties the supramolecular structures essentially determine photonic [1] and electric [2] material properties. One of the approaches to control the supramolecular structure is by means of interface assembly of dyes that have been made amphiphilic. This assembly is utilized in the Langmuir-Blodgett (LB) technique [3, 4] as well as in the Liquid-Liquid Interface Precipitate (LLIP) [2] technique. In our work we utilize both methods for the fabrication of model layers with tunable supramolecular structure for optoelectronic devices and self-healing membranes. This supramolecular structural tuning enables variation of the LUMO energy of fullerene films by 120 meV, that translate to 70 mV variation in open circuit voltage of corresponding pi-Si-hybrid solar cells [2].

[1] S. Das et al., ACS Appl Mater Interfaces, 2016, 8, 21512-21521.
[2] S. K. Das et al. Advanced Energy Materials, 2018, accepted.
[3] M. L. Hupfer et al., ACS Appl Mater Interfaces, 2017, 9, 44181-44191.
[4] M. Kaufmann et al., J. Colloid Interface Sci., 2018, 526, 410-418.

CPP 39.4 Wed 16:15 H14

In-situ study of printed films of PBDB-T-SF:IT-4F for application in organic solar cells — •Kerstin Wienhold[1], Volker Körstgens[1], Sebastian Grott[1], Xinyu Jiang[1], Matthias Schwartzkopf[2], Stephan Roth[2,3], 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, Sweden

Resent research in organic photovoltaics 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 device. However, towards commercialization, the solar cell performance must be optimized and an up-scale of the thin layer deposition is necessary. Printing of the active layer of organic solar cells can overcome the up-scale challenge. In-situ grazing incidence small angle X-ray scattering (GISAXS) during printing provides fundamental knowledge to better understand the drying kinetics and structure formation mechanism during printing. Characterization techniques such as UV/Vis spectroscopy, photoluminescence, optical microscopy and scanning electron microscopy (SEM) are applied after printing to get 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 39.5 Wed 16:30 H14

Simulation of active layer formation in solution-processed organic solar cells — •Olivier Ronsin and Jens Harting — Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg (IEK-11), Dynamics of Complex Fluids and Interfaces, Fürther Straße 248, 90429 Nürnberg, Germany

Solution-processed organic bulk-heterojunction active layers form sophisticated structures during the drying of the wet-deposited solution, because of complex physical processes such as crystallization and/or phase separation. This structure highly impacts the photovoltaic performance. In order to reach significant improvements, a better understanding of the physics driving the active layer formation is strongly needed.

We propose a phase-field simulation framework to determine the dry film structure. To this end, evaporation, crystal nucleation and growth, phase separation are taken into account as well as concentration-dependent diffusion coefficients. The model's behaviour for these basic physical processes will be shown, as well as simulation results for evaporation-induced phase separation and crystallization. First quantitative simulations for real photovoltaic systems and the comparison with in-situ experimental characterization on the drying structure will be presented.

CPP 39.6 Wed 16:45 H14

Inner structure analysis of quantum dot solids for photodevices — •Wei Chen and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Quantum dots (QDs) with near infrared emission are promising in both photodetectors (PDs) for sensing and photovoltaics (PVs) for solar energy conversion. High quality QDs are normally synthesized in solution and capped with organic ligands. To efficiently functionalize the QDs' array for PD or PV devices, the ligand exchange treatments, in solution or on solids, to colloidal QDs are necessary by exchanging or removing the long chain organic ligands. These treatments will not only decrease the inter-dot spacing between neighboring QDs to improve their electro-coupling behavior, which is beneficial for the energy transfer, but also change the stacking behavior of QD particles in solid from colloidal state to close packed state. This structure transition is now investigated by grazing incidence X-ray scattering and it is found that QDs prefer to stack in a face-centered cubic when they are in superlattice structure (colloidal state) by spin-coating. The stacking structure will change to a body-centered cubic style in a close packed solid after ligand exchange. Thus, the inner morphologies of QDs' close packed solids by different treatments are well studied. The optimized devices demonstrate a better device performances.

15 min. break

Invited Talk CPP 39.7 Wed 17:15 H14

Thin film structuring upon liquid-vapor mass exchange — •Jasper Michels — Max Planck Institute for Polymer Research, Mainz, Germany

Organic and hybrid thin film electronic devices, such as memory diodes, solar cells and transistors, typically contain a functional layer comprising a blend of polymeric or small-molecular species whose properties cooperatively give rise to a specific function. Depending on the desired device functionality, phase transitions during solution processing of these blends is either encouraged or suppressed. In many cases a microstructure evolves during solidification on account of, for instance, demixing or crystallization from solution. These processes may lead to drop-like or spherulitic structures, with associated feature sizes and domains shapes that depend on the processing conditions.

This presentation focuses on how phase separation couples with mass exchange across the liquid-vapor boundary, i.e. solvent evaporation and vapor condensation. I give an overview of the work we have done to understand the influence of liquid-vapor exchange rates on the dynamics of structure evolution. Modeling multi-component mixtures in the thermodynamic limit elucidates how microstructures evolve. Numerically simulated morphologies are consistent with experimentally observed ones and demonstrate in what way domain size and phase composition are affected by internal and environmental factors.

CPP 39.8 Wed 17:45 H14

Controlling Aggregate Formation in Conjugated Polymers by Spin-Coating Below the Critical Temperature of the Disorder Order Transition — •Anna Köhler — Soft Matter Optoelectronics and Bayreuth Institute of Macromolecular Research, University of Bayreuth, Germany

Aggregates, that is short-ranged ordered moieties in the solid-state of p-conjugated polymers, play an important role in the photophysics and performance of various optoelectronic devices. We have previously shown that many polymers change from a disordered to a more ordered conformation when cooling a solution below a characteristic critical temperature Tc. Using in situ time-resolved absorption spectroscopy on a range of semiconducting polymers including P3HT, PFO, PCPDTBT, and PCE11 (PffBT4T-2OD), we show that spincoating at a temperature below Tc can enhance the formation of aggregates with strong intra-chain coupling. An analysis of their time-resolved spectra indicates that the formation of nuclei in the initial stages of film formation for substrates held below Tc seems responsible for this. We observe that the growth rate of the aggregates is thermally activated with an energy of 310 meV, which is much more than that of the solvent viscosity (100 meV). From this we conclude that the rate controlling step is the planarization of a chain that is associated with its attachment to a nucleation center. The success of our approach for the rather dynamic deposition method of spin-coating holds promise for other solution-based deposition methods.

CPP 39.9 Wed 18:00 H14

Phase Formation Dynamics of Mixed-halide Perovskites by Real-time In-Situ Optical and X-ray Spectroscopy — •Justus Just[1], Klara Suchan[2], Pascal Becker[3], Eva Unger[2,3], and Thomas Unold[3] — [1]MAX IV Synchrotron Laboratory, Fotongatan 2, 22484 Lund, Sweden — [2]Lund University, Paradisgatan 2, 22350 Lund, Sweden — [3]Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

We present a detailed investigation of the phase formation dynamics of the chlorine derived one-step synthesis of $MAPbI_3$ perovskite. In a specially designed atmosphere controlled in-situ reactor, synchrotron based in-situ quick scanning X-ray absorption spectroscopy (QEXAFS), X-ray diffraction (XRD) as well as X-ray fluorescence (XRF) are applied in combination with in-situ optical reflection and photoluminescence spectroscopy. This enables us to correlate the evolution of the chemical reaction from XAS, the formation of crystalline phases from XRD and the chemical composition from XRF with the evolution of the optoelectronic properties of the film on one single timeline. We observe a delayed formation of crystalline $MAPbI_3$ and attribute it to a concentration threshold in the decreasing chlorine content of the sample. Our results give detailed insight into the formation process and can help to provide a mechanistic understanding of the reactions and intermediates involved. This knowledge can be utilized to optimize synthesis strategies and to tune the optoelectronic properties of organic-metal-halide perovskite semiconductors.

CPP 39.10 Wed 18:15 H14

On the colloidal behaviour of hybrid perovskite precursor dispersion and tracking structural heterogeneties arising from mixed perovskites: insights into the nano and macroscale — •Shambhavi Pratap[1,2], Johannes Schlipf[1], Kiran John[1], Volker Körstgens[1], Felix Fischer[1], Sundeep Vema[3], Alexander Holleitner[4], Anton Davydok[5], Christina Krywka[5], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Lawrence Berkeley National Laboratory, Advanced Light Source — [3]Cambridge University, Department of Chemical Engineering — [4]TU München, Walter Schottky Institut — [5]DESY, Helmholtz Zentrum Geesthacht, Hamburg

A colloidal nature of perovskite precursors 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. Morphological and structural heterogeneities within thin films are identified to be a consequence of deposition through dynamic precursors, far from thermodynamic equilibrium. The significance of such a finding suggests that perovskite films possess soft properties, implying there exists a delicate balance between entropic and enthalpic contributions towards the free energy of the dynamically changing system, which needs to be regulated for controlling film morphology; which has been established as a crucial prerequisite for improving solar cell performances.

CPP 39.11 Wed 18:30 H14

Following the perovskite crystallization in printed mesoscopic organometal halide perovskite solar cells — •Oliver Filonik[1], Margret Eva Thordardottir[1,2], Jenny Lebert[1], Stephan Pröller[1], Sebastian Weiss[1], Lew Jia Haur[3], Anish Priyadarshi[3], Nripan Mathews[3], Peter Müller-Buschbaum[2], and Eva M. Herzig[1,4] — [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

Printable perovskite solar cells based on carbon electrodes have shown outstanding device stability and upscalability in recent years. In this work, we follow the perovskite crystallization within the all-porous device architecture during fabrication and investigate the influence of the processing additive aminovaleric acid iodide (5-AVAI) on the perovskite formation. Using time-resolved grazing incidence wide angle X-ray scattering (GIWAXS), we are able to identify the suppression of large polycrystalline grains early in the fabrication process due to the processing additive. With the optimized processing conditions, an improved material backfilling and a significant device performance increase from (1.22 +- 0.03)% up to (10.69 +- 0.44)% is achieved. Our results grant us a better understanding of the initial perovskite crystallization phases and are of key importance for further developments.

CPP 40: Modeling and Simulation of Soft Matter I (joint session CPP/DY)

Time: Wednesday 15:00–17:00 Location: H18

CPP 40.1 Wed 15:00 H18

Thermodyanmics of Supramolecular Polymers with Hydrogen Bonding Ends — •Eunsang Lee and Wolfgang Paul — Institut für Physik, Marin-Luther-Universität Halle-Wittenberg, 06108 Halle, Germany

Rheological properties of supramolecular polymers (SMPs) depend on their equilibrium structure including the size, the number, and the topology of aggregates. In this work we investigate the thermodynamics of SMPs with H-bonding ends in a wide range of densities. Replica exchange stochastic approximation Monte Carlo simulations with coarse-grained models for polyethylene and polybuthylene glycols are used. Our heterocomplementary SMP system includes the same concentration of two different molecules, each of which is functionalized by different H-bonding stickers at both ends. Due to the chemical structure of sticker association, the functionality of the sticker varies depending on temperature, which is described by our H-bond potential and optimized parameters. Our simulation shows that SMPs have three transition lines with increasing temperature, a micelle (or gel)-ring transition, a ring-linear transition, and a linear-free chain transition. Because of the temperature-dependent functionality of the sticker, we can see the micelle (or gel)-ring transition at very low temperature which has not been observed in other associating polymers with fixed functionality. Below this transition line, the polymers in dilute concentration form flower-like micelles but polymers in semi-dilute concentration form a gel.

CPP 40.2 Wed 15:15 H18

Simulation of a large polymer with untruncated interaction near the collapse — •Stefan Schnabel and Wolfhard Janke — Universität, Leipzig

Off-lattice polymer models usually incorporate monomer-monomer interactions that act – at least in principle – at any distance. In consequence, calculating the energy and in particular the change in energy during a Monte Carlo move is typically an operation of computational complexity $\mathcal{O}(N^2)$, where N is the number of monomers. Since this complexity is inherited by the individual Monte Carlo move, only small polymers can be simulated without truncating the interaction potentials. We show how this can be avoided at temperatures near or above the collapse transition by using a Metropolis algorithm that tolerates inaccurate estimates of ΔE and present results for a polymer with Lennard-Jones interactions and $N \leq 65536$.

CPP 40.3 Wed 15:30 H18

Is there a universal equation of state for flexible polymers beyond the semi-dilute regime? — •Jaroslaw Paturej[1,2], Jens-Uwe Sommer[1], and Torsten Kreer[1] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]University of Szczecin, Szczecin, Poland

We reconsider the isothermal equation of state (EoS) for linear homopolymers in good solvents, $p = p(c, T)$, which relates the osmotic pressure, p, of polymers with the bulk concentration, c, and the temperature, T. The classical scaling theory predicts the EoS in dilute and semi-dilute regimes. We suggest a generalized EoS which extends the universal behavior of polymer solutions up to the highly concentrated state and confirmed it by molecular dynamics simulations and using available experimental data. Our conjecture implies that properties of polymer chains dominate the EoS in the presence of many-body interactions. Our theoretical approach is based on a viral expansion in terms of concentration blobs leading to a superposition of two power laws in the regime of concentrated solutions.

CPP 40.4 Wed 15:45 H18

Comparison of strain-induced transitions from liquid to solid of poly(ethylene oxide) and polyamide chains in water — •Sergii Donets[1], Olga Guskova[1], Gary Dunderdale[3], Oleksandr Mykhaylyk[3], 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 — [3]Department of Chemistry, University of Sheffield, Sheffield, S3 7HF, UK

Aqueous solutions of poly(ethylene oxide) (PEO) and polyamide oligomers are capable of undergoing a phase transition as a result of loss of the hydrated structure. Our simulations using an atomistic model 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 [1]. The strain-induced demixing transition from liquid to solid occurs primarily due to the favorable hydrophobic interactions in case of PEO chains and, in addition, due to the intermolecular hydrogen boding in case of polyamide chains. A tensile stress introduced into the aqueous solution 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 simulation box, leads to a phase separation from water. The strain-induced demixing of the extended chains provides the possibility to obtain polymer fibers with low energy costs.

[1] J. Phys. Chem. B, 2018, 122 (1), 392-397

CPP 40.5 Wed 16:00 H18

Soft deformable colloids: self-assembly and structure through computer simulations — •Mihir Khadilkar and Arash Nikoubashman — Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany

Colloids represent a rich class of soft materials that are important not only as model systems to study physical processes at nanoscale, but also as versatile building blocks towards a variety of technological applications. While hard-core models of colloids (with solely excluded volume interaction) have had great success in studying ordering, structure and dynamics in the past, most experimental systems exhibit varying degrees of softness that could potentially drastically alter their static and dynamic properties. Using molecular dynamics (MD) simulations of mesh models, we study the self-assembly of soft spherical and spheroidal colloids as a function of their elasticity and packing density. We quantify their arrangement and deformation using various order parameters. Further, we asses the dependence of eventual thermodynamic properties on the asphericity and softness of the colloids. For instance, we find that soft prolate ellipsoidal colloids (with aspect ratio 2) undergo a convex-to-concave transition at high pressures. The crystal structure also gets distorted, accompanied by an asymmetric deformation of principal directors. Addressing the structure-property relationship between softness arising from microstructure and the macroscopic properties could provide new routes towards designing and fabricating novel materials with tailored structural properties.

CPP 40.6 Wed 16:15 H18

Self-assembly of triblock terpolymers system using dissipative particle dynamic simulations — •Deepika Deepika and Arash Nikoubashman — Institute of Physics, Johannes Gutenberg University, Staudingerweg 7, 55128 Mainz, Germany

Self-assembly of triblock polymers into ordered structures has emerged as a promising technique for generating morphologies with nanometer range periodicity. The self-assembled structures dictated by the volume fraction of each block and interactions between them. In this work we are interested in the self-assembly behavior of polystyrene-polybutadiene-polymethyl-methacrylate (SBM) triblock copolymers in melt and in solution. The ternary phase diagram of SBM melt includes complex morphologies like spheres in lamellae cylinders in lamellae, cylinders in cylinder and many other. Equally intriguing is the solution phase behavior of SBM; recent experiments conducted by Groeschel et al. suggested ellipsoid aggregates of SBM in which layers of SBM are stacked in an ABCBA pattern. We conducted extensive DPD simulations to elucidate the effect of the process parameters, such as the volume fraction of each block and the Flory-Huggins interaction parameters, on the self-assembled structures. Our simulations give microscopic insights into the self-assembly behavior and provide useful design guidelines for fabricating structured nanoparticles in experiments.

CPP 40.7 Wed 16:30 H18

Construction of core-double-shell nanostructures via adsorption of mixed star polymers — •Qiyun Tang and Marcus Mueller — Institut für Theoretische Physik, Universität Göttingen

The adsorption of two kinds of star polymers with strongly adsorbing arm ends but distinct arm lengths onto one big gold nanoparticle results in the formation of a core-double-shell nanostructure. This radial-organized nanostructure finds potential applications in plasmonic and biomedical disciplines. Here we use theory and simulation to systematically study the formation process of this advanced nanostructure. Theoretical calculations predict that this structure does not reach equilibrium, but strongly depends on the formation kinetics. Simulation results show that the adsorption of short star polymers are chiefly dictated by diffusion whereas the adsorption of the end of a long star polymer implicates a high free-energy barrier generated by other chains, resulting in a protracted adsorption. The fabrication of the core-double-shell nanostructure is a combination of the diffusion-limited and the reaction-limited processes of short and long polymers, respectively, which is confirmed by experimental findings.

CPP 40.8 Wed 16:45 H18

Mixtures of Dendrimers and Linear Polymers — •Martin Wengenmayr[1,2], Ron Dockhorn[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]TU Dresden, Germany

One of the largely unsolved problems in polymer science is the effect of polymer architecture on the thermodynamics and functional properties of a polymer system. In particular, there is no commonly accepted explanation for the conformation properties of branched polymers immersed in a melt of chemically identical linear polymers. Based on Monte Carlo simulations of dendrimers with various generations and spacer lengths immersed in a solution of polymer chains of different degree of polymerization and concentrations we show that flexible dendrimers do not collapse into a compact globule as the concentration of linear chains is increased. Instead, we observe a crowded state distinct from athermal or theta solvent state. Beside the nontrivial conformational changes of the dendrimer the mixing of polymers of the same chemical composition but different branching induces secondary interactions between the species. Our work addresses the question of the strength of the secondary interactions in terms of intermolecular interactions and depletion attraction.

CPP 41: Charged Soft Matter, Polyelectrolytes and Ionic Liquids II

Time: Wednesday 15:00–15:30 Location: H13

CPP 41.1 Wed 15:00 H13

Neutron reflectivity and MD simulations of the silicon - deep eutectic solvent interface — •Nebojša Zec[1], Gaetano Mangiapia[1], Sebastian Busch[1], and Mikhail Zheludkevich[2] — [1]German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ) Helmholtz-Zentrum Geesthacht GmbH, 85748 Garching bei München, Germany — [2]Institute of Materials Research, Helmholtz-Zentrum Geesthacht, 21502 Geesthacht, Germany

The main aim of this work is to reveal the structure of the layers formed at the interface between deep eutectic solvents (DES) and silicon surface with and without applied constant electric potential using neutron reflectometry (NR) and molecular dynamics simulations (MDs). Work is focused on finding experimental evidence for an ordered layer of DES over an Si substrate under DC conditions and resolving the destruction of this layer by a superimposed AC field. Electrochemical experiments have shown that application of the potential of -1.6V superimposed with alternating sinusoidal component of 50 mV allows zinc depostion. Increasing temperature has the same effect and at 100 degrees C electrodeposition is possible even in potentiostatic regime. The results obtained with REFSANS instrument at Heinz Maier-Leibnitz Zentrum (MLZ) are compared with the reflectivity calculated from molecular dynamics simulations. Through this work we tend to determine the relationship between NR measurements of DES/silicon interface and the corresponding structural information obtained by MD simulations of the same system.

CPP 41.2 Wed 15:15 H13

Self-assembly of hollow colloidal silica cubes — •Margaret Rosenberg[1], Frans Dekker[2], Joe G. Donaldson[1], Albert P. Philipse[2], and Sofia S. Kantorovich[1,3] — [1]Department of Physics, University of Vienna, Vienna, 1090, Austria — [2]Van't Hoff Laboratory for Physical and Colloid Chemistry, Debye Institute for Nano-Materials Science, Utrecht University, NL — [3]Department of Mathematical Physics, Ural Federal University, Russia

Among the multitude of recently synthesized non-spherical colloids, hollow silica cubes distinguish themselves by their charged surface and the strong influence of van der Waals forces on their behaviour. While their self-assembly has been observed in experiment, it has not yet been fully studied and characterized. Using MD simulations, we investigate the electric double layer surrounding the cubes, then compute their interaction potential at different orientations to understand the influence of their anisometry. In combination with experimental observations and calculated trajectories, we show how the self-assembly of the cubes is driven by the competition between electrostatic and van der Waals forces. We then examine the microstructures formed by small clusters of cubes, which differ significantly from those exhibited by comparable spheres. These investigations give us a multifaceted understanding of the behaviour observed in these systems and pave the way for future applications.

CPP 42: Plasmonics IV (joint session O/CPP)

Time: Wednesday 15:00–17:45 Location: H8

CPP 42.1 Wed 15:00 H8

Switching between sharp Mie and broad plasmonic resonances in phase-change material metasurfaces — •Sophia Wahl, Andreas Hessler, Matthias Wuttig, and Thomas Taubner — Institute of Physics (IA) RWTH Aachen

Active metasurfaces (MSs) based on phase-change materials (PCMs) enable versatile compact optics like tunable metalenses [1]. PCMs can be rapidly and reversible switched between their amorphous and crystalline phases which is accompanied by a pronounced non-volatile change in their optical properties [2]. Commonly, PCMs integrated in MSs feature a large change in their positive permittivity.

We present how the phase-change material In_3SbTe_2 (IST) can be used to switch resonators in an infrared (IR) MS between sharp Mie resonances and broad plasmonic resonances. In the IR, the permittivity of IST changes from positive to negative upon crystallization, effectively switching from dielectric to metallic. We demonstrate how this can be used to dramatically change the resonance width and the resonance frequency of IR resonators.

Our work opens up new design concepts for applications like active spectral filters and absorbers, because it could provide tunable bandwidth and operation frequency at the same time.

[1] X. Yin et al., Light: Science & Applications 6, e17016 (2017)
[2] M. Wuttig et al., Nano Photon. 11, 465 (2017)

CPP 42.2 Wed 15:15 H8

Infrared nanoscopy to unravel the influence of defects in resistive switching of In_3SbTe_2 — •Niklas Eicker[1], Martin Lewin[1], Raimondo Cecchini[2], Sebastian Walfort[1], Matthias Wuttig[1], Martin Salinga[1], Massimo Longo[2], and Thomas Taubner[1] — [1]RWTH Aachen - Institute of Physics (1A) — [2]CNR - IMM

Phase change materials (PCMs) exhibit at least two stable states at room temperature, one crystalline and one amorphous. Characteristically the different states show a high electrical and optical contrast which can be used for fast, energy efficient and non-volatile nano switches [1]. Thus PCMs are a promising material class for persistent memory devices like PCRAM.

Scattering-type scanning near-field optical microscopy (s-SNOM) in the infrared spectral range can be used to study the differences in local conductivity of both states [2]. Opposed to other techniques like

TEM, SNOM allows to study the same system in different states without sample preparation or damaging the PCM.

To investigate the influence of defects on phase change processes in highly scaled PCM devices, we electrically contacted and switched PCM nanowires [3]. With infrared s-SNOM we revealed strong inhomogeneities, which might be linked to a reduced local conduction due to structural defects.

[1] M. Wuttig et al., Nat. Mater. 6, 824 (2007)
[2] M. Lewin et al., Appl. Phys. Lett. 107, 151902 (2015)
[3] S.Selmo et al., Appl. Phys. Lett. 109, 213103 (2016)

CPP 42.3 Wed 15:30 H8

Switchable absorber/emitter based on vanadium dioxide — •Xinrui Lyu[1,2,3], Taubner Thomas[1], and Yunzhen Cao[2] — [1]Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]Key Laboratory of Inorganic Coating Materials CAS, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 200050, PR China — [3]University of Chinese Academy of Sciences, Beijing 100049, PR China

We numerically demonstrate a switchable metamaterial absorber/emitter based on vanadium dioxide (VO2). The absorber consists of three layers, top patterned VO2 layer, dielectric spacer layer and bottom reflective layer. Perfect absorption can be thermally turned on when the excitation of magnetic resonance is supported with the metallic VO2, while switched off with semiconducting VO2. The absorption peak can be tuned with different shapes and geometries of patterned VO2 layer. The absorption bandwidth can be largely broadened when using lossy metallic VO2 instead of noble metal as reflective layer. The results would facilitate the design of switchable metamaterials for active control in energy and sensing applications.

CPP 42.4 Wed 15:45 H8

Tip-enhanced Raman spectroscopy of ultrathin ZnO layers on Ag(111) — •Shuyi Liu[1], Martin Wolf[1], and Takashi Kumagai[1,2] — [1]Department of Physical Chemistry, Fritz-Haber Institute of the Max-Planck Society, Faradayweg 4-6, 14195 Berlin, Germany. — [2]JST-PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan.

Tip-enhanced Raman spectroscopy (TERS) is a powerful nanoscale vibrational microspectroscopy combining high-spatial resolution of SPM with chemical sensitivity of surface enhanced Raman spectroscopy [1, 2, 3]. We report the TERS measurement of the ultrathin ZnO layers epitaxially grown on a Ag(111) surface. The enhancement mechanisms were examined in detail by a combination of STS and STM-induced luminescence spectroscopy with the TERS measurements. We found a clear correlation between the TERS signal and the plasmonic properties of the STM junction. It was also revealed that the TERS intensity increases exponentially with decreasing the tip-surface distance and the decay constant is largely different inside and outside the tunneling regime. Our results provide a detailed insights into the TERS mechanism and the plasmonic properties relevant for field enhancement and confinement in nanoscale cavities. References [1] Annu. Rev. Phys. Chem. 63, 379 (2012). [2] Chem. Rev., 117, 4961-4982 (2017) [3] Chem. Soc. Rev., 46, 4020 (2017).

CPP 42.5 Wed 16:00 H8

Dependence of graphene photoluminescence blinking on the local field enhancement — Markus Pfeiffer[1], •Mo Lu[1], Boris V. Senkovskiy[2], Danny Haberer[3], Felix R. Fischer[3], Fan Yang[2], Klaus Meerholz[1], Yoichi Ando[2], Alexander Grüneis[2], and Klas Lindfors[1] — [1]Department of Chemistry, University of Cologne, Luxemburger Str. 116, D-50939, Köln, Germany — [2]II. Physikalisches Institut, University of Cologne, Zülpicher Strasse 77, 50937 Köln, Germany — [3]Department of Chemistry, University of California at Berkeley, Tan Hall 680, Berkeley, CA 94720, USA

Armchair-edge graphene nanoribbons (AGNRs) are novel one-dimensional semiconductors with well-defined structure and promising optoelectronic properties. Their nanometer-sized dimensions and versatile electronic properties make them the ideal candidate for future optoelectronics. By coupling GNRs to plasmonic nanoantennas array, we obtain an enhancement of photoluminescence and Raman scattering intensity [1]. In the hotspots of the antennas, we observe the blinking of emission from AGNRs, which is a typical characteristic of a single quantum emitter [2]. Here we study the influence of the local field enhancement on the blinking process and find that the amplitude of the blinking events strongly correlates with the enhancement.

Reference:
[1] M. Pfeiffer, et al. 2D Materials, 5, 045006 (2018)
[2] M. Pfeiffer, et al. Nano Lett. 18, 7038-7044 (2018)

CPP 42.6 Wed 16:15 H8

Electrochemistry on Copper Nanostructures for Active Plasmonics — •Annette Böhme, Florian Sterl, Elinor Kath, Monika Ubl, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Applications of active plasmonics include the development of advanced plasmonic color displays and switchable metasurfaces. We aim to fabricate plasmonic nanostructures that can be switched electrochemically by applying a voltage.

Copper is a suitable material for this attempt as it can easily be switched electrochemically between copper (Cu) and copper oxide (CuO/ Cu$_2$O) [1]. We have developed a manufacturing process to fabricate high-quality inverse copper nanostructures that exhibit well-modulated plasmonic resonances. We use these samples to perform cyclic voltammetry in order to switch them electrochemically, and at the same time we perform spectral reflectance measurements in the visible wavelength range. Thereby, we demonstrate that the resonances can be reversibly shifted by as much as 80 nm. The wavelength shift becomes stronger after several cycles of voltammetry which we attribute to the modification of the copper surface with repeated oxidation and reduction.

These results provide a basis for the future development of pixelated active plasmonic devices.

[1] Ye Wan, Yundian Zhang, Xianle Wang, and Qing Wang, Electrochem. Commun. 36, 99 (2013).

CPP 42.7 Wed 16:30 H8

How Metal Nanoantennas' Optical Properties Affect Surface Enhanced Infrared Absorption — •Michael Tzschoppe, Christian Huck, Jochen Vogt, Frank Neubrech, and Annemarie Pucci — Kirchhoff Institute for Physics, Heidelberg University, Germany

Surface enhanced infrared absorption (SEIRA) is known as a powerful tool to study tiny amounts of molecules on the basis of enhanced vibrational signals. In order to further increase the enhancement, the impact of the structures' geometry as well as their interaction have been intensively investigated within the last decade.[1,2] We present an experimental study with focus on the impact of the nanoantennas' metal-optical properties on SEIRA sensitivity. Various aspect ratios of nanoantennas made of the metals gold, silver, copper, aluminum, and iron, respectively, were inspected. From the measured fundamental plasmonic resonance spectra the contributions of the intrinsic damping (electron scattering) as well as the radiative damping (light scattering) were evaluated. The SEIRA enhancement factors were determined for a thin organic probe layer. These investigations finally yield the correlation between the ratio of intrinsic damping and radiation damping with the SEIRA enhancement, which clearly shows the maximum enhancement when both damping mechanisms contribute equally.[3]

[1] Neubrech *et al.* Chem. Rev. **2017**, 117 (7), 5110
[2] Dong *et al.* Nano Lett. **2017**, 17 (9), 5768
[3] Tzschoppe *et al.* J. Phys. Chem. C **2018**, 122 (27), 15678

CPP 42.8 Wed 16:45 H8

Watching a single fluorophore molecule walk into a plasmonic hotspot — Ling Xin[1,2], •Mo Lu[3], Steffen Both[4], Markus Pfeiffer[3], Maximilian J. Urban[1,2], Chao Zhou[1,2], Hao Yan[5], Thomas Weiss[4], Na Liu[1,2], and Klas Lindfors[3] — [1]Max Planck Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany — [2]Kirchhoff Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany — [3]Department of Chemistry, University of Cologne, Luxemburger Straße 116, 50939 Köln, Germany — [4]4th Physics Institute and Stuttgart Research Center of Photonic Engineering, University of Stuttgart, 70569 Stuttgart, Germany — [5]Department of Chemistry & Biochemistry, Biodesign Institute, Arizona State University, Tempe, AZ 85287-5601, USA

Plasmonic nanoantennas allow for enhancing the spontaneous emission, altering the emission polarization, and shaping the radiation pattern of quantum emitters. A critical challenge for the experimental realizations is positioning a single emitter into the hotspot of a plasmonic antenna with nanoscale accuracy. We demonstrate a dynamic light-matter interaction nanosystem enabled by the DNA origami technique. A single fluorophore molecule can autonomously and unidirectionally walk into the hotspot of a plasmonic nanoantenna along a designated origami track. Successive fluorescence intensity increase and lifetime reduction are in situ monitored using single-molecule fluorescence spectroscopy. Our scheme offers a dynamic platform, which can be used to develop functional materials, investigate intriguing light-matter interaction phenomena as well as to serve as examine theoretical models.

CPP 42.9 Wed 17:00 H8

Surface-enhanced infrared absorption spectroscopy for in-vitro detection of the polypeptide monolayer conformation on a single gold nanoantenna — •Rostyslav Semenyshyn[1,2], Florian Mörz[1,2], Frank Neubrech[1,3], and Harald Giessen[1,2] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart — [2]Center for Integrated Quantum Science and Technology, IQST — [3]Kirchhoff Institute for Physics, University of Heidelberg

In our present work, we demonstrate the capability of surface-enhanced infrared absorption spectroscopy for ultra-sensitive in-vitro detection of the secondary structure of polypeptides monolayer. We utilized a monolayer of thiols as a bonding spacer for deposition of poly-L-lysine (PLL) molecules onto the gold surface [1]. We tuned the length of nanoantennas to be resonant at the frequency of the amide-I band of PLL and performed SEIRA measurements in the D_2O environment using a specially designed transmittance flowcell. To measure an optical response of a *single* nanostructure, we pushed our system towards the diffraction limit and therefore applied a light source with higher brilliance, namely specifically designed broadband tunable laser [2]. Then, we compare our results to a globar, as well as a synchrotron, which are well-known FTIR light sources. With further advances it might become possible to scale the process down to a few or even single proteins.
[1] R. Semenyshyn, M. Hentschel, C. Stanglmair, T. Teutsch, C. Tarin, C. Pacholski, H. Giessen, and F. Neubrech, Nano Lett. (2018); doi: 10.1021/acs.nanolett.8b02372 [2] T. Steinle, F. Mörz, A. Steinmann, and H. Giessen, Opt. Lett. 41, 4863 (2016)

CPP 42.10 Wed 17:15 H8

Optical Nanoplasmonic CO2 Detection in the Visible by Polyethylenimine — •Pohl Tobias, Sterl Florian, Strohfeldt Nikolai, and Giessen Harald — 4th Physics Institute and Research Center SCOPE, University of Stuttgart, 70569 Stuttgart, Germany

In industrial production and other technologically relevant processes CO2 is a common byproduct that must be monitored to keep up a high efficiency. Most of the currently available CO2 detection systems use an electrical readout. This poses in environments with explosive or flammable gases a major risk of spark ignition. The available optical solutions, which circumvent this risk altogether, rely on the characteristic infrared absorption of CO2. While being very specific this method requires a large sensing volume. In our contribution, we introduce a cheap and compact nano-optical gas detection scheme for CO2 based on a plasmonic perfect absorber structure combined with the polymer polyethylenimine. The polymer acts as the gas sensitive part as it changes its refractive index by absorbing CO2, which is then translated by the absorber to a resonance shift. By tracking the plasmon resonance we studied the time, concentration, and temperature dependence, as well as possibilities to enhance the response and aging effects. Furthermore we will show that this sensing scheme also works with a much simpler setup consisting only of a LED, a photodiode, and appropriate electronics.

CPP 42.11 Wed 17:30 H8

three-dimensional plasmonic nanostructure design for boosting photoelectrochemical — •rui xu, huaping zhao, max sommerfeld, and yong lei — Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693, Ilmenau, Germany

Plasmonic nanostructures have been widely incorporated into different semiconductor materials to improve solar energy conversion. An important point is how to manipulate the incident light so that more light can be efficiently scattered and absorbed by the semiconductors. Here, by using a tunable three-dimensional Au pillar/truncated-pyramid (PTP) array as a plasmonic coupler, a superior optical absorption of about 95% within a wide wavelength range is demonstrated from an assembled CdS/Au PTP photoanode. Based on incident photon to current efficiency measurements and the corresponding simulations, it is concluded that the enhancement is mainly attributed to an appropriate spectral complementation between surface plasmon resonance modes and photonic modes in the Au PTP structure over the operational spectrum. Because both of them are wavelength dependent, the Au PTP profile and CdS thickness are further adjusted to take full advantages of the complementary effect and subsequently, an angle independent photocurrent with an enhancement of about 400% was obtained. The designed plasmonic PTP nanostructure of Au is highly robust and it could be easily extended to other plasmonic metals equipped with semiconductor thin film for photovoltaic and photoelectrochemical cells.

CPP 43: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge VI (joint session O/DS/CPP/TT)

Time: Wednesday 15:00–17:45 Location: H9

CPP 43.1 Wed 15:00 H9

First-principles quantum transport simulations including strong correlation effects — •Andrea Droghetti[1], Wilhelm Appelt[2], Liviu Chioncel[2], Milos Radonjić[3], Enrique Muñoz[4], Stefan Kirchner[5], David Jacob[1], Dieter Vollhardt[2], Angel Rubio[6], and Ivan Rungger[7] — [1]University of the Basque Country (Spain) — [2]University of Augsburg (Germany) — [3]University of Belgrade (Serbia) — [4]Pontificia Universidad Católica de Chile — [5]Zhejiang University (China) — [6]Max Planck Institute for the Structure and Dynamics of Matter (Germany) — [7]National Physical Laboratory (UK)

When magnetic molecules are brought into contact with metals the electron-electron interaction leads to the appearance of the correlated Kondo state. In this talk we will present the results of first-principles calculations for the electronic structure and the linear-response conductance of radical molecules adsorbed on metallic surfaces in the Kondo regime [Phys. Rev. B 95, 085131 (2017), Nanoscale 10, 17738 (2018)]. In particular we will outline the methodological approach as implemented in the Smeagol electron transport code and we will benchmark the results against experiments. The method relies in the first place on the combination of Density Functional Theory with the Green's functions technique. We will explain how a molecular devices is projected onto an effective Anderson impurity problem, which is then solved either by continuum time quantum Monte Carlo or numerical renormalization group. Finally, we will describe some work-in-progress aimed at computing transport properties beyond linear-response.

CPP 43.2 Wed 15:15 H9

Density functional theory for transport through correlated systems — •Stefan Kurth — Univ. of the Basque Country UPV/EHU, San Sebastian, Spain — IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — Donostia International Physics Center DIPC, San Sebastian, Spain

A recently proposed density functional formalism to describe electronic transport through correlated systems in the steady state uses both the density on the junction and the steady current as basic variables. The corresponding Kohn-Sham system features two exchange-correlation (xc) potentials, a local xc potential and an xc contribution to the bias, which are universal functionals of the basic variables.

A recent parametrization of the xc potentials for the single-impurity Anderson model correctly incorporates both the Kondo and Coulomb blockade regimes. It allows for calculation of currents and differential conductances at arbitrary bias and temperature at negligible numerical cost but with the accuracy of sophisticated renormalization group methods. A time-local version of this functional is used to study the Anderson model under the influence of both DC and AC biases. We observe interaction-induced shifts of the photon-assisted conductance peaks, supression of the Kondo plateau at zero temperature and lifting of Coulomb blockade at finite temperature.

CPP 43.3 Wed 15:30 H9

Exact factorization of the many-electron wave function — •Camilla Pellegrini[1], Antonio Sanna[1], and Eberhard K. U.

Gross[1,2] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany — [2]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

The exact factorization approach [1], originally developed for a system of electrons and nuclei, is extended to a system of electrons only. This allows for a two-particle Schroedinger equation, which uniquely defines the exact effective interaction between two electrons in the medium. This interaction differs from the effective interaction, W, used in many-body Green's function techniques. In particular, it is spin-dependent. We illustrate the formalism for the simplest case of exchange interactions only.

[1] A. Abedi, N.T. Maitra, E.K.U. Gross, PRL 105, 123002 (2010).

CPP 43.4 Wed 15:45 H9

Many-body spectral functions from steady state density functional theory — •David Jacob[1,2] and Stefan Kurth[1,2,3] — [1]Dpto. de Física de Materiales, Universidad del País Vasco UPV/EHU, San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [3]DIPC, San Sebastián, Spain

We present a scheme to extract the true many-body spectral function of an interacting many-electron system from an equilibrium density functional theory (DFT) calculation [1]. To this end we devise an ideal STM-like setup and employ the recently proposed steady-state DFT formalism (i-DFT) which allows to calculate the steady current through a nanoscopic region coupled to two biased electrodes [2]. In our setup one of the electrodes serves as a probe ("STM tip"). In the ideal STM limit of vanishing coupling to the tip, the system to be probed is in quasi-equilibrium with the "substrate" and the normalized differential conductance yields the exact equilibrium many-body spectral function. Moreover, from the i-DFT equations we derive an exact relationship which expresses the interacting spectral function in terms of the Kohn-Sham one. Making use of i-DFT xc functionals that capture Coulomb blockade as well as Kondo physics, the method yields spectral functions for Anderson impurity models in good agreement with NRG calculations. It is thus possible to calculate spectral functions of interacting many-electron systems at the cost of an equilibrium DFT calculation.

References: [1] D. Jacob and S. Kurth, Nano Lett. **18**, 2086 (2018) [2] G. Stefanucci and S. Kurth, Nano Lett. **15**, 8020 (2015)

CPP 43.5 Wed 16:00 H9

Magnetic phase transitions induced by pressure and magnetic field: the case of antiferromagnetic USb2 — •Leonid Sandratskii — Max Planck Institute of Microstructure Physics, Halle, Germany

Fascinating phenomena observed under applied pressure and magnetic field are currently attracting much research attention. Recent experiments have shown that application of the pressure or magnetic field to the USb2 compound induce the transformations of the ground-state antiferromagnetic (AFM) up-down-down-up structure to, respectively, ferromagnetic (FM) or ferrimagnetic configurations. Remarkably, the magnetic critical temperature of the FM state, induced by pressure, is more than two times smaller than the Neel temperature of the ground state. We performed density-functional theory (DFT) and DFT+U studies to reveal the origin of the unusual magnetic ground-state of the system and the driving mechanisms of the phase transitions. We investigate both the magnetic anisotropy properties and the parameters of the interatomic exchange interactions. To study pressure-induced effects we carry out calculations for reduced volume and demonstrate that the AFM-FM phase transformation indeed takes place but depends crucially on the peculiar features of the magnetic anisotropy. We also explain why the magnetic field that couples directly to the magnetic moments of atoms leads to the phase transition to the ferrimagnetic state whereas the pressure that does not couple directly to magnetic moments results in the FM structure.

CPP 43.6 Wed 16:15 H9

Charge localization at a weakly coupled molecule-metal system studied by linear expansion Δ-self-consistent field density-functional theory (ΔSCF-DFT) — •Hadi H. Arefi[1,2], Daniel Corken[3], Reinhard Maurer[3], F. Stefan Tautz[1,2], and Christian Wagner[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]Department of Chemistry, University of Warwick, Coventry, United Kingdom

Predicting the charge arrangements at the interface between molecules and metals represents a formidable challenge for semi-local approximations to Density Functional Theory (DFT). This could become even more critical when molecules are only weakly coupled to the metal. Single-molecular devices based on such weak coupling have recently been created by molecular manipulation with a scanning probe microscope (SPM), where a single PTCDA (perylene-tetracarboxylic dianhydride) molecule was placed in a free-standing upright configuration either on a SPM tip [1] or on a pedestal of two adatoms on the Ag(111) surface [2]. There are indications that the mechanism stabilizing these unexpected configurations is linked to an integer charge transfer creating a singly occupied molecular orbital. We use the ΔSCF-DFT method [3] to confine charge on the LUMO of the PTCDA and study the consequences with vdW-corrected DFT.

[1] C. Wagner et al. Phys. Rev. Lett. 115, 026101 (2015) [2] T. Esat et al. Nature 558, 573 (2018) [3] R. J Maurer, K. Reuter, JCP 139, 014708 (2013)

CPP 43.7 Wed 16:30 H9

Dispersion corrected density functional theory studies on PVDF/hydrated aluminium nitrate composite system — •Ranjini Sarkar and Tarun Kundu — Indian Institute of Technology, Kharagpur

Electro-active polymer Polyvinylidene fluoride (PVDF) based ferroelectric composites have gained significant technological importance over conventional ceramic ferroelectrics. This article provides quantum chemical description of PVDF/ hydrated aluminium nitrate salt composite system in the light of density functional theory. Four monomer units of pristine α and β-PVDF, pure Al(NO3)3.9H2O, and PVDF/ Al(NO3)3.9H2O structures are optimized using dispersion corrected exchange correlation functional B3LYP-D and 6-311+G(d,p) basis set. Similar to the experimental findings, the current theoretical investigation also suggests that hydrogen bond interaction between PVDF and the hydrated salt molecule plays the major role for the enhancement of ferroelectric properties in this composite system. Non-covalent interaction phenomenon is elucidated on the basis of natural bond orbital analysis, Bader's quantum theory of atoms in molecules and reduced density gradient analysis. Chemical Reactivity and charge transfer mechanisms are explained using atomic-dipole corrected Hirshfeld population analysis, molecular electrostatic potential plot and frontier molecular orbital analyses, respectively.

CPP 43.8 Wed 16:45 H9

Band-structure effects in vertical layered material heterostructures — •Nicholas D. M. Hine[1], Gabriel C. Constantinescu[2], Nelson Yeung[1], Siow-Mean Loh[1], José María Escartín[2], Cuauhtemoc Salazar Gonzalez[1], and Neil R. Wilson[1] — [1]Department of Physics, University of Warwick, United Kingdom — [2]Cavendish Laboratory, University of Cambridge, 19 JJ Thomson Avenue, Cambridge CB3 0HE, United Kingdom

Controlling the properties of layered material heterostructures is crucial to the success of devices based on the novel capabilities of 2D materials, yet theoretical insight has been limited by the large system sizes required to study rotated, incommensurate interfaces. We use linear-scaling DFT calculations with non-local vdW functionals to explore large-scale models of heterostructures of interest for device applications. Results will be presented for heterostructures including MoS2/MoSe2, MoSe2/WSe2, and other Transition Metal Dichalcogenide pairings, TMDCs with graphene and hBN substrates, and hBN/Phosphorene. Band-structure changes caused by stacking and rotation of the layers are obtained by unfolding the supercell spectral function into the primitive cells, incorporating spin-orbit coupling. Changes in spectral weight and band-structure between the monolayers and heterostructured interfaces show how lattice mismatch (MoS2/MoSe2) or spacer layers (Phosphorene/hBN/Phosphorene) can allow the component monolayers to retain more independence in heterostructures than in homo-stacks. Finally, applying electric fields allows the behaviour of gated structures to be predicted and explained.

CPP 43.9 Wed 17:00 H9

Global Trends in Calcium-Silicate-Hydrate Phases Identified by Infrared Spectroscopy and Density Functional Theory — •Mohammadreza Izadifar, Franz Königer, Andreas Gerdes, Christof Wöll, and Peter Thissen — Karlsruhe Institute of Technology (KIT), Institute of Functional Interfaces (IFG), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Building and construction industry are at the same time the backbone and the driving force of our modern society. Nearly all our today's technical infrastructure is based on cement-based materials. Detailed, spectroscopic investigations of model reactions on well-defined mineral substrates under UHV-conditions are largely lacking, thus prohibiting a validation of theoretical methods. Eight different Calcium-Silicate-Hydrate (CSH) phases, namely Tobermorite 14Å, Tobermorite 11Å, and Tobermorite 9Å, Wollastonite, Jaffeite, Jennite, γ-C2S, and α-C2SH, are calculated with the help of Density Functional Theory using the Vienna ab initio simulation package (VASP). First, we take care of the mechanical properties of the material. Our results revealed that Jaffeite, γ-C2S, and α-C2SH have a linear bulk modulus due to the monomer structure of silicate tetrahedra. Tobermorite 14Å and Jaffeite have the lowest and highest bulk modulus, respectively. In the second part, the optimized geometries allow for the precise calculations vibrational eigenmodes and frequencies by the force-constant (FC) approach. The proportions of C/S and H/C are major criteria for the classification of the calculated wavenumber of ν(Si-O) for all phases in our model system.

CPP 43.10 Wed 17:15 H9

Origin of carbon 1s binding energy shifts in amorphous carbon materials — •Michael Walter[1,4,5], Filippo Mangolini[2], Robert W. Carpick[3], and Michael Moseler[4,5] — [1]FIT, University of Freiburg, Germany — [2]University of Texas at Austin, USA — [3]University of Pennsylvania, USA — [4]Fraunhofer IWM, Freiburg, Germany — [5]Physikalisches Institut, Universität Freiburg, Germany

The quantitative evaluation of the carbon hybridization state by X-ray photoelectron spectroscopy (XPS) has been a surface-analysis problem for the last three decades due to the challenges associated with the unambiguous identification of the characteristic binding energy values of sp^2- and sp^3-bonded carbon. Here, we compute the binding energy values for model structures of various carbon allotropes, including graphite, diamond, doped-diamond, and amorphous carbon (a-C), using density functional theory (DFT). The large band-gap of diamond allows defects to pin the Fermi level, which results in large variations of the C(1s) core electron energies for sp^3-bonded carbon, in agreement with the large spread of experimental C(1s) binding energy values for sp^3 carbon. In case of hydrogen-free a-C, the C(1s) core electron binding energy for sp^3 carbon atoms is approximately 1 eV higher than the binding energy for sp^2-hybridized carbon. However, the introduction of hydrogen hinders the unambiguous quantification of the carbon hybridization state on the basis of C(1s) XPS alone. This work can assist surface scientists in the use of XPS for the accurate characterization of carbon-based materials.

CPP 43.11 Wed 17:30 H9

Mechanically tuned conductivity of graphene grain boundaries from first-principles calculations — Delwin Perera, •Jochen Rohrer, and Karsten Albe — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Nanocrystalline graphene has recently been shown to have a strong piezoresistivity and strain gauge factors that are notably higher compared to single- or microcrystalline graphene [1]. The origin of the enhanced piezoresistivity in nanocrystalline graphene is still not fully understood, but several theoretical works suggest that grain boundaries are the main cause as these can evoke transport gaps.

In our work we test this assumption with density functional theory based transport calculations of graphene bicrystals. In particular, we extend our analysis of the interplay between grain boundary structure and transport properties [2] by including mechanical strain. We compute transmission functions and current-voltage curves and compare them with tight binding calculations. Our findings suggest that the strain-induced transport gap modulation can be fully described by the response of the bulk graphene band structure towards strain.

[1] Riaz *et al.*, Nanotechnology **26**, 325202 (2015)
[2] Perera *et al.*, Phys. Rev. B **98**, 155432 (2018)

CPP 44: Condensed-matter simulations augmented by advanced statistical methodologies (joint session DY/CPP)

Time: Wednesday 15:00–18:45 Location: H20

Invited Talk CPP 44.1 Wed 15:00 H20

Quantum Machine Learning — •Anatole von Lilienfeld — Institute of Physical Chemistry, University of Basel

Many of the most relevant chemical properties of matter depend explicitly on atomistic and electronic details, rendering a first principles approach to chemistry mandatory. Alas, even when using high-performance computers, brute force high-throughput screening of compounds is beyond any capacity for all but the simplest systems and properties due to the combinatorial nature of chemical space, i.e. all compositional, constitutional, and conformational isomers. Consequently, efficient exploration algorithms need to exploit all implicit redundancies present in chemical space. I will discuss recently developed statistical learning approaches for interpolating quantum mechanical observables in compositional and constitutional space. Results for our models indicate remarkable performance in terms of accuracy, speed, universality, and size scalability.

CPP 44.2 Wed 15:30 H20

Quantum Monte Carlo method for Vibrational Frequencies — •Yu Yang Liu and Gareth Conduit — University of Cambridge, UK

Quantum Monte Carlo methods have become a leading contender for high accuracy calculations for the electronic structure. Calculating energy derivatives such as atomic forces and the matrix of force constants is important in relaxing structures, calculating vibrational properties, and performing molecular dynamics simulations. We develop a quantum mechanical expectation value to evaluate the matrix of force constants directly in Quantum Monte Carlo. The approach allows the full modeling of correlation effects such as Van der Waals force, opening new applications to molecules and solids in condensed matter.

CPP 44.3 Wed 15:45 H20

Localized Basis Functions for Variationally Enhanced Sampling — •Benjamin Pampel, Kurt Kremer, and Omar Valsson — Max Planck Institute for Polymer Research, Mainz, Germany

Variationally Enhanced Sampling (VES) is a recently developed method for molecular dynamics simulations. It enhances sampling by introducing a bias potential along certain collective variables that is constructed via minimisation of a convex functional.

This bias potential is usually represented by a linear expansion in some basis set, with delocalised functions such as plane waves or Chebyshev/Legendre polynomials as common choices. However, it is an open question if localised functions perform better. In particular, the wavelet family of Daubechies might be a good choice. These functions offer the favourable property of forming an orthonormal basis with a tunable number of vanishing moments. Furthermore, their intrinsic principle of multiresolution allows increasing the precision of the bias representation at specific points of interest.

We have implemented Daubechies wavelets into the VES code and have tested their performance in various systems. As a direct comparison of the different basis sets is difficult, we have developed a new measure of the error of free energy calculations. The Daubechies wavelets are observed to perform better than both Chebyshev/Legendre polynomials and Gaussian basis functions, resulting in faster convergence and yielding more accurate free energy surfaces without increases in computational cost.

CPP 44.4 Wed 16:00 H20

Representing molecules and materials for accurate interpolation of quantum-mechanical calculations — •Marcel Langer, Alex Goessmann, and Matthias Rupp — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

The search for novel materials, the exploration of phase diagrams and other high-throughput applications require numerical simulations of molecules and materials from first principles, but are limited by their high computational cost. By interpolating between reference calculations, machine learning can act as a fast accurate surrogate for these calculations, greatly increasing the number of accessible systems. [1]

This requires a *representation* of molecules and materials suitable for interpolation. We show how the state-of-the-art representations can be understood in a unified framework [2] based on local descriptions of atomic environments via k-body functions, group averaging and tensor products, and discuss implications. We benchmark predictive accuracy of selected representations by carefully controlling for all other factors, including data distribution, regression method and optimization of free parameters. For the latter, we employ a consistent and fully automatic procedure to optimize both numerical and categorical free parameters, such as the choice of k-body functions, using sequential model-based optimization with tree-structured Parzen estimators. [3]

References: [1] a) Rupp et al, Phys Rev Lett **108**, 058301, 2012. b) Rupp, Int J Quant Chem **115**, 1058, 2015. [2] Willatt et al, Phys Chem Chem Phys, accepted, 2018. [3] a) Bergstra et al, NIPS **24**, 2546, 2011; b) Bergstra etal, ICML **30**, I-115, 2013.

CPP 44.5 Wed 16:15 H20

Machine Learning of Free Energies — •Clemens Rauer and Tristan Bereau — Max Planck Institute for Polymer Science, Ackermannweg 10, 55128 Mainz, Germany

Free energies are important molecular properties which can provide an insight into the thermodynamic state of the respective system. Accurate calculations of free energies are an important tool for many biophysical applications, ranging from protein-ligand binding[1] to the insertion of small molecules into a lipid[2]. However, computationally expensive high level simulations are necessary in order to obtain accurate free energy estimates, and therefore, only a small subset of chemical space can be accurately covered. We overcome this problem by building a Δ-machine learning[3] model. Using this approach we can use a "cheap" low level method to predict free energies and learn the correction to a higher level method or experimental value. Then, we can predict high level free energies for significantly larger compound sets than was used in the training of the model. We show that by using only limited high level data, highly accurate free energies can be calculated using this method. As a first system we apply this approach to the prediction of hydration free energies.

[1] Mobley, D.L. & Gilson, M.K. *Annu. Rev. Biophys.* **2017**, 46:531-58

[2] Menichetti, R. et al. *J. Chem. Phys.* **2017**, 147, 125101

[3] Ramakrishnan et al. *J. Chem. Theory Comput.* **2015**, 11, 2087-2096

CPP 44.6 Wed 16:30 H20

Deep Learning for Multiscale Simulations of Soft Matter Systems — •Marc Stieffenhofer[1], Tristan Bereau[1], and Michael Wand[2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz — [2]Institute of Computer Science, Johannes Gutenberg University Mainz

The great success of Deep Neural Networks (DNNs) is based on their ability to learn and extract descriptive features directly from training data and to build a hierarchical, abstract representation of the input that takes multiple length scales into account. Such multiscale representations can also be found in soft matter systems where many physical phenomena and properties are governed by a large range of different length- and timescales.

In this work, we explore links between multiscale representations of DNNs and multiscale simulations of soft matter systems. The main focus is to investigate if DNNs can be used to link distribution functions generated at different resolutions. We have applied DNNs to the backmapping of coarse-grained molecular configurations to higher-resolution representations. This requires to reproduce the fine-grained statistics that match the coarse-grained representation.

Our model relies on 3D convolutional neural networks that are trained to generate molecular equilibrium structures. The training of the model is based on the generative adversarial approach and results are discussed for a system of octane molecules.

CPP 44.7 Wed 16:45 H20

Unsupervised machine learning of chemical compound space for hierarchical screening and coarse-graining applications — •Kiran Kanekal, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Recently, the number and type of chemical fingerprints used for supervised learning of molecular properties has increased significantly, as the importance of properly encoding the 3D structure of a molecule to greatly increase accuracy has been recognized. Some of the most successful of these fingerprints encode a great deal of physical information, including coefficients for potential energy functions commonly used in classical atomistic molecular dynamics simulations [1]. In this work, we incorporate these fingerprints into an unsupervised machine learning (clustering) scheme to define subspaces in the chemical compound space, for which we use the Generated DataBase [2] (GDB) as a proxy. We show that the use of different molecular fingerprints leads to significant differences in the clustering observed, as each fingerprint will highlight specific molecular properties. Therefore, unsupervised learning, when coupled with these fingerprints, naturally enables hierarchical screening approaches for materials design. Furthermore, the presence of strong correlations between clusters identified using different fingerprints implies that a lowering of resolution (i.e. coarse-graining) is viable for that specific region of chemical compound space.

1. B. Huang and O. A. von Lilienfeld, J. Chem. Phys. 2016, 145, 161102. 2. T. Fink and Jean-Louis Reymond, J. Chem. Inf. Model. 2007, 47, 342.

15 min. break

CPP 44.8 Wed 17:15 H20

Understanding three-body contributions to coarse-grained force fields — •Christoph Scherer, Rene Scheid, Tristan Bereau, and Denis Andrienko — Max-Planck-Institut für Polymerforschung, Mainz, Germany

Coarse-graining (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 [1]. The CG scheme is implemented in the VOTCA-CSG toolkit [2]. 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 of the Stillinger-Weber type having a significant two-body component. This interference can be alleviated by CG the two-and three-body contributions separately. Furthermore, we employ Kernel-based Machine learning (ML) [3] overcoming the restrictions of a fixed basis set. The approach is illustrated on liquid water where three-body interactions are essential to reproduce the structural properties, and liquid methanol where two-body interactions are sufficient to reproduce the main features of the atomistic system. [1] Scherer, Andrienko, PCCP, 20, 22387 (2018); [2] Rühle, Junghans, Lukyanov, Kremer, Andrienko, JCTC, 5, 3211 (2009); [3] Glielmo, Sollich, De Vita, PRB, 95, 214302 (2017)

CPP 44.9 Wed 17:30 H20

Reweighting Dynamics of Nonequilibrium Steady States — •Marius Bause, Timon Wittenstein, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz

Markov State Models(MSM) are a discrete representation of the kinetics of a given system constructed by coarse-graining microtrajectories. While frequently applied to equilibrium systems, a protocol for non-equilibrium steady state systems (NESS) has not been developed due to loss of dynamic properties like detailed balance. We propose to apply the principle of Maximum Caliber by Jayne's, postulating that the distribution of paths is given by the maximal path entropy. The markovian assumption alleviates the combinatorial explosion of microtrajetories. The entropy production between states is chosen for a physical constraint and defines the NESS ensemble. By choosing a reference system for a prior, reweighting between ensembles becomes possible. The entropy productions become the defining elements of the ensemble. The method is tested on a minimal model under non-conservative forces.

CPP 44.10 Wed 17:45 H20

Free Energy Landscape of Phase Transitions Investigated by Enhanced Sampling over Degenerate Collective Variables — •Bin Song, Kurt Kremer, and Omar Valsson — Max Planck Institute for Polymer Research, Mainz, Germany

Phase transition events such as nucleation of atomic or molecular crystals, self-assembly of micelles etc. have been intriguing scientists not only for their underlying physical principles, but also for their potential applications. Molecular dynamic simulations are increasingly called upon to either provide the detailed mechanistic insights and to prognosticate such events that may be too expensive or slow to examine with experiments. As potential energy surface of such events are often complex and difficult to sample, free energy surface (FES) are preferred. However, FES presents its own challenge to sample when the height of barriers are higher than or comparable to the thermal energy. Enhanced sampling methods biasing on properly chosen collective variables (CVs) can help overcome these barriers. Sometimes globally defined CVs are not sufficient, and more than a few of locally defined ones are needed. The increased dimensionality of the bias potential could be another source of frustration for achieving properly sampled FES, which we would like to alleviate with our new development of Variational Enhanced Sampling (VES) in cases where the local CVs are permutationally invariant. We demonstrate the capability of the new development by sampling the phase transitions in systems of increased complexity, including Lennard-Jones clusters and liquid-solid transition in materials.

CPP 44.11 Wed 18:00 H20

Efficient Equilibration of Hard Particles with Collective Moves – A Comparison of Computational Methods — •Marco Klement and Michael Engel — Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen, Germany

Particle simulations are an important method to study the phase behavior of fluids and solids. A common task is structure prediction via thermal equilibration. Examples are crystallization or melting and the aging of glasses. Near the liquid-solid phase transition of hard spheres event driven molecular dynamics is known as most efficient. Monte Carlo simulations are boosted by event-chain in the same region. It is neither clear how equilibration does benefit from Newtonian motion nor how the efficiency of an algorithm should be quantified; and several ways are in use. Here we present further improvement of event-chain Monte Carlo by bringing the chain closer to natural movement with particle reflection events and quantify the improvement using different approaches from literature.

CPP 44.12 Wed 18:15 H20

The temperature dependence of the mechanical unfolding of a supramolecular complex studied by molecular simulations — Takashi Kato, Ken Schäfer, Stefan Jaschonek, and •Gregor Diezemann — Institu für Physikalische Chemie, Universität Mainz

The conformational dynamics of supramolecular complexes can be studied on a single molecule level using the techniques of dynamic force spectroscopy and important kinetic information can be extracted. Using models for the free energy landscape of the system as a function of the molecular extension it is possible to obtain parameters like the bare unfolding rate, the activation free energy in the force-free case and also the distance between the folded configuration and the transition state. In the present work we performed molecular simulations of the mechanical unfolding of a model molecular complex, a pair of interlocked calixarene catenanes. From rupture force distributions the kinetic rates for the opening transition were extacted for varying parameters of the pulling device. In order to be able to perform a model-free analysis we performed simulations over a broad range of temperatures and found Arrhenius behavior for the kinetic rates. This allows to determine the activation free energy and the bare rate independently as a function of the force without using specific models for the shape of the energy landscape. We discuss our findings in light of the models that are usually used in the analysis of force dependent kinetic rates obtained from experimental or simulation data.

CPP 44.13 Wed 18:30 H20

An efficient anharmonic free energy method applied to vacancies in ZrC — •Thomas Mellan[1], Andrew Duff[2], Blazej Grabowski[3], and Michael Finnis[1] — [1]Imperial College, London, UK — [2]Hartree Centre, Daresbury, UK — [3]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

We have developed a thermodynamic integration approach to calculate the anharmonic contribution to the volume and temperature dependent free energy of a crystal. The method provides an effective balance between accuracy and computational efficiency, giving a factor of 15 speed-up on comparable free energy approaches with average errors less than 1 meV/atom. The method is demonstrated with new predictions on the thermodynamics of substoichiometric ZrC, including vacancy concentration and heat capacity.

CPP 45: Photovoltaics (joint session HL/CPP)

Time: Wednesday 15:00–17:30 Location: H36

CPP 45.1 Wed 15:00 H36

Revisiting the electronic structure of vanadium doped In_2S_3 — •Elaheh Ghorbani[1], Paul Erhart[2], and Karsten Albe[1] — [1]Institut für Materialwissenschaft, Technische Universität Darmstadt, Darmstadt, Germany — [2]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

Transition metal impurities often have noticeable impacts on the electronic and optical properties of the host material. Recently, they have been suggested as intentional dopants for the purpose of creating intermediate metallic bands within the band gap of parent semiconductor. These intermediate bands (IB), if partially filled and optimally placed between valence and conduction bands, can collect photons of sub-band gap energies and enhance the photocurrent density. In this context, the formation of an IB in V-doped In_2S_3 (In_2S_3:V) was predicted by first-principles calculations. In this contribution, we revisit In_2S_3:V, using a band gap corrected method (hybrid functional) and show that V^{3+} (with $3t_{2g}^2e_g^0$ configuration) substituting for octahedral In^{3+} is a Jahn-Teller active ion. The aroused Jahn-Teller distortion necessitates removing the degeneracy of t_{2g} levels through splitting it into filled e and empty a sublevels, which reside at the top of the valence band and bottom of the conduction band, respectively. Consequently, no IB forms, when both V and In are in 3+ oxidation state. To give a fuller picture of In_2S_3:V, we studied the rehybridization of V d orbitals with S p orbitals for different oxidation numbers of V. Our results show that in the presence of a reducing agent, like H^+, a totally filled t_{2g} level can form inside the gap.

CPP 45.2 Wed 15:15 H36

Angle-resolved electroreflectance spectroscopy on CIGS solar cell absorber and buffer layers — •Jasmin Seeger[1], Jonas Grutke[1], Wolfram Witte[2], Dimitrios Hariskos[2], Oliver Kiowski[2], Heinz Kalt[1], and Michael Hetterich[1,3] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70563 Stuttgart, Germany — [3]Light Technology Institute, KIT, 76131 Karlsruhe, Germany

Thin-film Cu(In,Ga)Se_2 (CIGS) solar cells can be further improved by replacing the standard CdS buffer layer with an alternative material, which leads to less absorption losses and therefore higher efficiencies. We employ electroreflectance spectroscopy (ER) for the destruction-free determination of the bandgap energies of different buffer materials grown by chemical bath deposition and to get insights into potential interdiffusion processes at the buffer/absorber interface. In this contribution, a new ER technique called angle-resolved electroreflectance spectroscopy (ARER) is presented, which allows the determination of the buffer's bandgap energy. This is possible despite interference effects occurring due to the layered structure and despite the low signal due to the small buffer thickness. To demonstrate the applicability of ARER, results for absorber and CdS buffer layers are shown and compared to results from other ER measurement methods. Additionally, ARER is applied to solar cells with Zn(O,S) buffer layers, enabling the determination of the sulfur to oxygen ratio of the Zn(O,S) buffer and yielding hints for the possible formation of mixed phases.

CPP 45.3 Wed 15:30 H36

Spatially resolved composition and functionality of high efficiency Cu(In,Ga)Se2 thin film solar cells — •Christian Plass[1], Maurizio Ritzer[1], Philipp Schöppe[1], Sven Schönherr[1], Philip Jackson[2], Roland Wuerz[2], Claudia S. Schnohr[1], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, Stuttgart, Germany

Cu(In,Ga)Se2 solar cells yield one of the highest efficiencies among all thin film photovoltaics. Compositional variations of the absorber elements as well as incorporated alkali elements significantly affect the conversion efficiency. Hence there is a strong need to determine the composition spatially resolved.

High resolution synchrotron based methods like X-ray fluorescence analysis (XRF) and X-ray beam induced current (XBIC) enable insight into such compositional and functional variations. Simultaneous XRF and XBIC measurements of complete solar cells were conducted in plan-view geometry: The highly focused X-ray nanobeam at the ID16B-NA station of the European Synchrotron Radiation Facility scanned the solar cell and by analyzing the emitted X-Ray fluorescence radiation together with the corresponding induced current correlating maps are obtained. As the spatial resolution is about 50 nm, we can show how different elemental compositions, grains and grain boundaries influence the measured current.

CPP 45.4 Wed 15:45 H36

Intrinsic point defects in kesterite-type Cu$_2$ZnGeSe$_4$ compound semiconductors — •Daniel Fritsch[1] and Susan Schorr[1,2] — [1]Department Structure and Dynamics of Energy Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Department of Geosciences, Freie Universität Berlin, Malteserstr. 74-100, 12249 Berlin, Germany

In recent years, kesterite-type compound semiconductors such as Cu$_2$ZnSnS$_4$ and Cu$_2$ZnSnSe$_4$ (CZTSSe) received a lot of attention due to their possible application as absorber layers in low-cost thin-film solar cells. However, substituting Ge^{4+} for Sn^{4+} in CZTSSe kesterite-type absorber layers has been shown to improve the optoelectronic properties [1].

Here, we address the computational modelling of intrinsic point defects in kesterite-type Cu$_2$ZnGeSe$_4$ employing density functional theory together with the PBE and the more accurate hybrid functional HSE06. Details of the intrinsic defects' characteristics will be discussed, as well as their influence on the electronic and optical properties.

This work made use of computational resources provided by the North-German Supercomputing Alliance (HLRN), and the Soroban and Dirac HPC facilities of the Freie Universität Berlin and the Helmholtz-Zentrum Berlin, respectively.

[1] R. Gunder, J. A. Márquez-Prieto, G. Gurieva, T. Unold, and S. Schorr, Cryst. Eng. Comm. **20**, 1491 (2018).

15 min. break

CPP 45.5 Wed 16:15 H36

2D sb2s3 periodic structure induced absorption enhancement — •Wei Wang, Patrick Pfeiffer, and Lukas Schmidt-Mende — Konstanz University

Sb2S3 is a promising candidate for solar cell absorbers due to its high absorption coefficient, suitable band gap and earth-abundant constituents. Here we present the fabrication of 2D Sb2S3 structures by direct laser interference method and direct electron beam lithography method. The periodic structure induced absorption enhancement can be observed by UV-VIS absorption spectrum and verified by finite difference time domain (FDTD) simulation.

CPP 45.6 Wed 16:30 H36

Numerical and experimental analysis of the time resolved photo-luminescence method at the buffer-absorber interface of CIGS thin film solar cell — •Ashwin Hariharan, Ievgeniia Savchenko, Jörg Ohland, Hippolyte Hirwa, and Stephan Heise — LCP, University of Oldenburg, Oldenburg, Germany

The minority carrier lifetime is an important second level parameter which affects the primary parameters of the solar cell. To study the minority carrier lifetime - or more generally, the carrier dynamics -, time-resolved photoluminescence (TRPL) method is a powerful technique. The main result obtained from TRPL is the luminescence decay time (or in some cases more than one decay constant), after which two questions follow: (i) under which circumstances is the decay time a direct indicator of minority carrier lifetime, and (ii) is the correlation between minority carrier lifetime and open-circuit voltage valid across all cases. The primary objective of this research is to understand the first correlation in a more perfect manner by studying the charge carrier separation near the heterojunction of CdS/CIGSe. The study includes both experimental analysis and simulation using, Synopsys TCAD. Experimentally, the main analysis involves wavelength-dependent pulsed illumination through which one gains control of the carrier injection density at different depths inside the absorber layer. For simulation, accurate representation of material parameters in the space charge region of the junction will be done. Based on the baseline model, dependence between physical parameters must be found in order to establish the agreement between numerical and experimental decay curves.

CPP 45.7 Wed 16:45 H36

The impact of solar cell layer variations on the temperature coefficient of CIGS thin film solar cells — •Hamsa Ahmed[1], Janet Neerken[1], Jörg Ohland[1], Ievgeniia Savchenko[1], Hippolyte Hirwa[1], Alfons Weber[2], Robert lchner[2], Jürgen Parisi[1], and Stephan Heise[1] — [1]University of Oldenburg, D-26111 Oldenburg, Germany — [2]Avancis GmbH, Munich, Germany

One of the most promising alternatives in photovoltaic technologies is Cu(In,Ga)(S,Se)2 (CIGS)-based thin *lm solar cells, mainly because it has reached over 22% efficiency during the recent years, its high energy yield production, and relatively low temperature coefficients (βx). The temperature coefficients quantify how the solar cell performance changes with temperature and they play a significant role to maximize the energy yield. In order to investigate the impact of the individual solar cell layers on the temperature coefficients, in this study a systematic characterization was performed on various CIGS solar cells with different layer variations such as the absorber, back contact, and buffer layer. The temperature coefficients were extracted from IV (current-voltage) measurements indoor at different illumination intensities in the range of (20*50)°C. Low temperature IV measurements were accomplished in order to assess the activation energies, and to compare them with the band gap values from glow-discharge optical emission spectroscopy (GDOES) and external quantum efficiency (EQE) measurements. Further analyses were accomplished to examine the recombination; such as thermal admittance spectroscopy (TAS) to correlate it with the diode parameters n and J0.

CPP 45.8 Wed 17:00 H36

The impact of solar cell layer variations on the temperature coefficient of CIGS thin film solar cells — •Hamsa Ahmed[1], Janet Neerken[1], Jörg Ohland[1], Ievgeniia Savchenko[1], Hippolyte Hirwa[1], Alfons Weber[2], Robert lchner[2], Jürgen Parisi[1], and Stephan Heise[1] — [1]University of Oldenburg, D-26111 Oldenburg, Germany — [2]Avancis GmbH, Munich, Germany

One of the most promising alternatives in photovoltaic technologies is Cu(In,Ga)(S,Se)2 (CIGS)-based thin film solar cells, mainly because it has reached over 22% efficiency during the recent years, its high energy yield production, and relatively low temperature coefficients (βx). The temperature coefficients quantify how the solar cell performance changes with temperature and they play a significant role to maximize the energy yield. In order to investigate the impact of the individual solar cell layers on the temperature coefficients, in this study a systematic characterization was performed on various CIGS solar cells with different layer variations such as the absorber, back contact, and buffer layer. The temperature coefficients were extracted from IV (current-voltage) measurements indoor at different illumination intensities in the range of (20*50)°C. Low temperature IV measurements were accomplished in order to assess the activation energies, and to compare them with the band gap values from glow-discharge optical emission spectroscopy (GDOES) and external quantum efficiency (EQE) measurements. Further analyses were accomplished to examine the recombination; such as thermal admittance spectroscopy (TAS) to correlate it with the diode parameters n and J0.

CPP 45.9 Wed 17:15 H36

2D sb2s3 periodic structure induced absorption enhancement — •Patrick Pfeiffer, Wei Wang, and Lukas Schmidt-Mende — Konstanz University

Sb2S3 is a promising candidate for solar cell absorbers due to its high absorption coefficient, suitable band gap and earth-abundant constituents. Here we present the fabrication of 2D Sb2S3 structures by direct laser interference method and direct electron beam lithography method. The periodic structure induced absorption enhancement can be observed by UV-VIS absorption spectrum and verified by finite difference time domain (FDTD) simulation.

CPP 46: Microswimmers (joint session DY/CPP)

Time: Wednesday 15:30–18:00 Location: H19

CPP 46.1 Wed 15:30 H19

Orientational ordering and collective motion in (semi-)dilute suspensions of active microswimmers — Christian Hoell, Giorgio Pessot, Hartmut Löwen, and •Andreas M. Menzel — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

Polar orientational ordering in crowds of self-propelled particles is connected to the emergence of collective motion. We study orientational ordering in suspensions of active microswimmers. These objects propel by setting the surrounding fluid into motion. Since we focus on (semi-) dilute suspensions, such hydrodynamic effects dominate the swimmer interactions. For simplicity, we concentrate on planar arrangements of so-called pushers and pullers, which induce different flow fields.

In such a situation, our simulations indicated polar orientational ordering for puller microswimmers, in contrast to pushers [1]. Thus, we analyzed the behavior of binary pusher–puller mixtures. Interestingly, we found that smaller amounts of pusher microswimmers can show a larger degree of orientational order than surrounding puller microswimmers in an ordered suspension of mainly pullers [1]. Increasing the amount of pushers makes the orientational order break down.

To further quantify these phenomena, we performed a linear stability analysis of a corresponding dynamical density functional theory for pusher and puller suspensions [2]. Indeed, we found homogeneous polar orientational order to arise from a linear instability of disordered suspensions of strong pullers, in contrast to pushers.

[1] G. Pessot et al., *Mol. Phys.* **116**, 3401 (2018).
[2] C. Hoell et al., *J. Chem. Phys.* **149**, 144902 (2018).

CPP 46.2 Wed 15:45 H19

Maximum in density heterogeneities of active swimmers — •Fabian Jan Schwarzendahl[1] and Marco G. Mazza[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]Interdisciplinary Centre for Mathematical Modelling and Department of Mathematical Sciences, Loughborough University, Loughborough, Leicestershire LE11 3TU, United Kingdom

Suspensions of unicellular microswimmers such as flagellated bacteria or motile algae can exhibit spontaneous density heterogeneities at large enough concentrations. 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. By employing multiparticle collision dynamics, we directly couple the swimmer's dynamics to the fluid's. 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 the competition of hydrodynamic and steric interactions between swimmers. We develop an analytical theory that supports these results. This maximum might represent an optimum for the microorganisms' colonization of their environment.

CPP 46.3 Wed 16:00 H19

Stabilization of a square vortex lattice in microswimmer suspensions by periodic arrays of obstacles — •Henning Reinken[1], Sebastian Heidenreich[2], Igor S. Aranson[3], Markus Bär[2], and Sabine H.L. Klapp[1] — [1]Technische Universität Berlin, Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [3]Pennsylvania State University, University Park, PA 16802, USA

Bacterial suspensions, a paradigmatic example of an active fluid, are known to exhibit a state denoted as mesoscale turbulence which is characterized by chaotic dynamics of vortices of a characteristic size. In a recent experiment, these vortices have been stabilized into a square lattice with antiferromagnetic order by geometrically constraining the bacterial suspension using periodic arrays of obstacles with a spacing in the range of the unconstrained vortex size [1]. Interestingly, the vortices are consistently located in the gaps between the obstacles rather than forming around them [1]. We aim to reproduce the patterns observed in the experiment using a recently derived fourth-order field theory for a vectorial order parameter representing an effective microswimmer velocity [2]. In this continuum theoretical framework, we numerically explore different implementations of the constraints: Obstacles that favor negatively charged topological defects straightforwardly reproduce the observed vortex lattice configuration. For topologically neutral defects, higher order nonlinear effects are required to break the topological symmetry and stabilize a certain configuration.

[1] D. Nishiguchi et al., Nat Commun. **9**, 4486 (2018).
[2] H. Reinken et al., Phys. Rev. E **97**, 022613 (2018).

CPP 46.4 Wed 16:15 H19

Complex dynamic response of magnetocapillary swimmers — •Alexander Sukhov[1], Sebastian Ziegler[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, P.O. Box 513, NL-5600MB Eindhoven, The Netherlands

Using the lattice Boltzmann method and the Shan-Chen model for multiple fluid components we simulate an interface with several rigid magnetic particles floating on it. The stability of the system is reached when the attractive capillary forces resulting from the weights of the particles are balanced by the repulsive magnetic forces induced by an external static magnetic field applied perpendicularly to the interface. The particles can propel themself at the interface when a smaller oscillating magnetic field of the right frequency is applied in the plane of the interface. We aim at understanding the contributions of interparticle and hydrodynamic interactions as well as that of the interface to the dynamic response of the swimmer when simulating a single, two and three particles at the interface separately.

CPP 46.5 Wed 16:30 H19

Microswimmers in an axisymmetric vortex flow: from Hamiltonian dynamics to clustering — •José-Agustín Arguedas-Leiva and Michael Wilczek — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Microswimmers appear in a wide variety of settings, ranging from phytoplankton in the ocean to bacteria in laboratory flows, and are known to give rise to many physically interesting phenomena. One such phenomenon is the clustering of otherwise neutrally buoyant particles. Its occurrence, and in particular the importance of physical parameters such as particle shape and swimming velocity, are currently not fully understood.

Here, we study the the distribution and clustering of swimmers in a two-dimensional axisymmetric vortex flow. Due to its simplicity, this system allows for a number of insights: We find that spherical swimmers follow phase-space preserving Hamiltonian dynamics, excluding the possibility for clustering. Interestingly, changing the particles' shape breaks the Hamiltonian structure of the dynamics, and clustering can occur. Based on this observation we identify a single control parameter: an effective swimming velocity, which takes into account both the particles' shape and velocity. By characterizing the topology of the underlying phase space our results help to clarify the role of motility and shape-dependent hydrodynamic interactions.

15 min. break

CPP 46.6 Wed 17:00 H19

Oscillatory dynamics of swimming E. coli bacteria in wall-bounded Poiseuille flow — •Andreas Zöttl[1,2], Arnold Mathijssen[1,3], Nuris Figueroa-Morales[2], Gaspard Junot[2], Éric Clément[2], and Anke Lindner[2] — [1]University of Oxford, UK — [2]ESPCI Paris, France — [3]Stanford University, USA

Swimming microorganisms respond to flows in highly diverse and complex environments, at scales ranging from open oceans to narrow capillaries. The combined effects of fluid flow and boundaries lead to preferred swimmer orientation breaking the up/down-stream and left/right symmetry. To date, this so-called bacterial surface rheotaxis has been quantified by measuring instantaneous orientation distributions or average transport velocities, but a complete picture is still missing.

We investigate the time-resolved orientation dynamics of E.coli bacteria, theoretically and experimentally, as a function of applied shear close to walls. With increasing flow, we identify four regimes separated by critical shear rates: (I) circular swimming with a bias along the direction of vorticity; (II) upstream swimming without oscillations; (III) oscillatory motion, increasingly more to the left; (IV) coexistence of swimming to the left and to the right, with dynamical switching between these states. By modeling bacterial rheotaxis comprehensively - accounting for their chiral nature, hydrodynamic and steric interactions, elongation, fore-aft asymmetry and activity - we assess the relative importance of these contributions throughout a trajectory, and explain the full dynamics.

CPP 46.7 Wed 17:15 H19

Polarization of Brownian swimmers with spatially heterogeneous activity — •Sven Auschra[1], Nicola Söker[2], Paul Cervenak[1], Viktor Holubec[1], Klaus Kroy[1], and Frank Cichos[2] — [1]Institute for Theoretical Physics, University of Leipzig, 04103 Leipzig, Germany — [2]Peter Debye Institute for Soft Matter Physics, University of Leipzig Leipzig, 04103 Leipzig, Germany

Janus particles fuelled by laser heating are paradigmatic autophoretic microswimmers. Their dynamics under constant driving has been well characterized [1-3]. We consider situations in which the particles' propulsion strength fluctuates in space and time, due to a variable fuel supply. Specifically, we analyze their spatial and orientational distribution experimentally, realizing prescribed spatial and temporal activity variations via the laser heating. We find depletion in regions of higher activity and polarization in activity gradients. Using Brownian dynamics simulations and a powerful numerical solver for Fokker-Planck equations [4], we can reproduce the experimental observations. A simple run-and-tumble process captures the observed features, qualitatively, and provides some analytical insights.

[1] A. Bregulla and F. Cichos: Faraday Discuss. 184, 381-391 (2015)
[2] H. Jiang, N. Yoshinaga, and M. Sano: PRL 105, 268302 (2010)
[3] A. Würger: Rep. Prog. Phys. 73, 126601 (2010)
[4] V. Holubec, K. Kroy and S. Steffenoni: arXiv:1804.01285v2 (2018).

CPP 46.8 Wed 17:30 H19

Efficiency limits of the three-sphere swimmer in viscous fluids — •Babak Nasouri[1], Andrej Vilfan[1,2], and Ramin Golestanian[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Göttingen, Germany — [2]J. Stefan Institute, Ljubljana, Slovenia — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, United Kingdom

We consider a swimmer consisting of a collinear assembly of three spheres connected by two slender rods. This swimmer, as first shown by Najafi and Golestanian (Phys. Rev. E 69, 062901 2004), can propel itself forward by varying the lengths of the rods in a way that is not invariant under time reversal. Although any non-reciprocal strokes of the arms can lead to a net displacement, the energetic efficiency of the swimmer is strongly dependent on the details and sequences of these strokes. We define the efficiency of the swimmer using Lighthill's criterion, i.e., the power that is needed to pull the swimmer by an external force at a certain speed, divided by the power needed for active swimming with the same average speed. Here, we determine numerically the optimal stroke sequences while limiting the maximum extension of the rods. Our calculation takes into account both far-field and near-field hydrodynamic interactions. We specifically show that the swimming efficiency initially rises by increasing the maximum allowable extension of the rods, and then converges to a maximum value.

CPP 46.9 Wed 17:45 H19

Actuation of particles in modulated Poiseuille flow — •Winfried Schmidt[1,2], Matthias Laumann[1], Eva Kanso[2], and Walter Zimmermann[1] — [1]Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Aerospace and Mechanical Engineering, University of Southern California, Los Angeles, USA

What is the dynamical behavior of micro-particles in Poiseuille flow with oscillating flow direction at low Reynolds number? We investigate the overdamped motion of bead-spring models, e.g., capsules and red blood cells. We predict net motion of the particles, despite vanishing mean flow. This effect is generic as it does not depend on the model and is explained by a broken symmetry. The mean actuation velocity of passive particles is caused by their varying shape in both half periods. Since the net velocity depends also on the size and the elasticity of the particles, this novel actuation mechanism is appropriate for particle sorting. The system is also explored for active particles.

CPP 47: Complex Fluids and Soft Matter (joint session DY/CPP)

Time: Wednesday 15:00–19:15 Location: H3

Invited Talk CPP 47.1 Wed 15:00 H3

Phase-separation in an elastic matrix: from living cells to synthetic materials — •Eric Dufresne — ETHZ

In order to function effectively, living cells need to compartmentalize myriad chemical reactions. In the classic view, distinct functional volumes are separated by thin oily-barriers called membranes. Recently, the spontaneous sorting of cellular components into membraneless liquid-like domains has been appreciated as an alternate route to compartmentalization.

I will review the essential physical concepts underlying these phenomena and outline some of the fundamental questions in soft matter physics that they inspire. Then, I will describe our recent experiments exploring the impact of mechanical stresses on the condensation of droplets. This work spans experiments with living cells and synthetic polymer networks, with an eye toward useful new materials.

CPP 47.2 Wed 15:30 H3

Breakup of a particulate suspension jet — •Joris Chateau[1,2] and Henri Lhuissier[1] — [1]CNRS, Aix-Marseille University, Marseille, France — [2]Max Planck Institute, Gottingen, Germany

As viscosity is increased, a liquid capillary jet accelerated by gravity stretches over increasingly large distances before eventually breaking up. This Newtonian behavior is profoundly altered for particulate suspensions. Adding solid particles to a liquid, which increases the effective viscosity, can paradoxically shorten the jet considerably. This apparent contradiction is rationalized by considering finite size effects occurring at the scale of a few particles. A model is presented which captures the breakup length of suspension jets observed experimentally for a broad range of liquid viscosities, particle sizes and extrusion velocities of the jet, and recovers the Newtonian case for vanishing particle sizes. These results can be readily extended to any stretched jet configuration and potentially to other fluid media having a granularity.

CPP 47.3 Wed 15:45 H3

Self-assembly and dynamics of mixtures of magnetic and non-magnetic liquid crystals under shear and external magnetic field — •Nima H. Siboni, Gaurav P. Shrivastav, and Sabine H. L . Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36 D-10623 Berlin

Doping liquid crystals with magnetic particles of different shapes enables us to control the properties of this delicate phase of matter via an external magnetic field [1,2]. In this talk, we focus on mixtures where the magnetic particles have the same shape as the liquid crystals. We study the self-assembly and dynamics of the mixture in and out of equilibrium [3]. In particular, we utilize non-equilibrium molecular dynamics simulation of Gay-Berne particles [4] to study (i) the (composition-dependent) effect of an external magnetic field on the isotropic-to-nematic transition of the mixture, and (ii) the interplay between shear-induced order and the magnetic field-induced order on the mechanical response of the mixture to an applied external shear.

References:
[1] I. Dierking, and S. E . San, Appl. Phys. Lett. **87**, 233507 (2005).
[2] G. P. Shrivastav, and S. H. L. Klapp, arXiv:1809.08288.
[3] N. H. Siboni, G. P. Shrivastav, and S. H. L. Klapp, *in preparation.*
[4] J. G. Gay, and B. J. Berne, J. Chem. Phys., **74**, 3316 (1981).

CPP 47.4 Wed 16:00 H3

Marangoni flow in thin freely suspended liquid films — •Torsten Trittel[1], Christoph Klopp[1], Kirsten Harth[2], Alexey Eremin[1], and Ralf Stannarius[1] — [1]Institute for Physics, Otto von Guericke University, 39106 Magdeburg — [2]Physics of Fluids and Max Planck Center for Complex Fluid Dynamics, P.O. Box 217, 7500 AE Enschede

Next to their great success in display applications, liquid crystals are enormously attractive in the field of fundamental physics. Freestanding films with unique aspect ratios can serve as an ideal system for the investigation of two-dimensional hydrodynamics. We focus on thermocapillary effects in such films under microgravity. We present results of two suborbital rocket flights and show that thermal gradients within the film plane can cause thermocapillary (Marangoni) effects. The temperature dependence of the surface tension $\sigma(T)$ can induce flow from the hot to the cold film edge. Finally we developed a hydrodynamic model that can describe the experimental observations quantitatively. In contrast to Benard-Marangoni or Rayleigh-Benard convection, the relevant control parameter is the temperature difference, not the temperature gradient across the film.

The study was supported by the German Aerospace Center (DLR) within projects 50WM1430 and 50WM1744.

CPP 47.5 Wed 16:15 H3

Shear-waves from cavitation in soft solids — •Julien Rapet[1,2], Yoshiyuki Tagawa[3], and Claus-Dieter Ohl[1,2] — [1]Nanyang Technological University, Singapore — [2]Otto-Von-Guerricke Universität, Magdeburg, Germany — [3]Tokyo University of Agriculture and Technology, Tokyo, Japan

While the fluid mechanics of cavitation is a mature research area, very little is known for bubbles undergoing large and non-spherical volume changes in a soft elastic solid. Here soft solids made from gelatin-water mixtures mimic tissue. Previous studies demonstrated that the collapse of a bubble entrapped in soft solids emits longitudinal waves at the speed of sound. Yet the elasticity of the medium supports also transversal waves propagating at a considerable lower speed. We show how cavitation in elastic solids may lead to the emission of such shear waves, particularly the collapse of bubbles near an air/solid interface. The cavitation bubbles are obtained by focusing a pulsed laser into the tissue mimicking material. The bubble dynamics and shear wave propagation are observed with high-speed imaging and photoelastic imaging, respectively. We show that similar to water the cavity moves during collapse away from the free surface accelerating a jet in the direction of the bubble's center of mass motion. During this process the volume between the air/solid interface and the bubble is sheared. Yet the dynamics is much faster than the shear wave speed and therefore the shear stress remains confined. For sufficiently strong and non-spherical collapses, the gelatin surface deforms and a crack starting from the interface propagating towards the bubble.

CPP 47.6 Wed 16:30 H3

Self-organized lattices and coalescence of droplets in freely suspended liquid crystal films — •Christoph Klopp[1], Torsten Trittel[1], Kirsten Harth[2], Alexey Eremin[1], and Ralf Stannarius[1] — [1]Otto von Guericke University, Institute for Physics, 39106 Magdeburg, Germany — [2]Universiteit Twente, Physics of Fluids and Max Planck Center for Complex Fluid Dynamics, 7500 AE Enschede, The Netherlands

Colloids in freely suspended smectic films are an excellent system to study self-organisation in restricted (2D) dimensionality. The dynamics of the colloids in such films is fully 2D. We demonstrate the formation of two-dimensional hexagonal lattices of isotropic droplets stabilized by repulsive interactions in freely suspended films [1]. The dynamics of single droplets in a six-neighbor cage can be described using the Saffman model for mobility in a 2D fluid. We show that the modified model reproduces the experimental observations, the droplet mobility in the lattice depends only on the ratio of cage and droplet sizes, irrespective of droplet sizes. At higher temperatures, droplets coalesce. Droplets on free-standing films have the shapes of flat lentils and their coalescence dynamics are expected to be intermediate between 2D and 3D cases [3]. We measured the coalescence which is on a time scale of milliseconds depending on the radii of the involved droplets.

[1] Clark N., et al., 2017. Adv. Space. Res. 60 737

[2] Eremin, A., Baumgarten, S., Harth, K., Stannarius, R., 2011. Pys. Rev. Lett. 107, 268301.

[3] Hopper R., 1984, J. Am. Ceram. Soc. 67, C-262

CPP 47.7 Wed 16:45 H3

Re-entrant) Splashing of drops impacting on a heated plate at reduced pressure — •Kirsten Harth, Michiel van Limbeek, Paul Hoefnagels, and Detlef Lohse — Physics of Fluids, Max Planck Center and Universiteit Twente, Enschede, The Netherlands

Splashing drops capture our minds with their fascinating beauty - and splash control is highly relevant in a wide range of applications involving impacting drops. It is thus not surprising that diverse criteria for the splash threshold have been put forward over the last decades, with a recent breakthrough by Riboux and Gordillo (e.g. PRL 113 189901 (2014)). The effect of the surrounding gas is included via the mean free path, thus the theory also captures the disappearance of upon decrease of the ambient pressure. In our present understanding, identical drops remain intact at low impact velocities, while they always splash above a critical velocity.

Drop impact on heated surfaces in reduced pressure, however, bears a counterintuitive surprise: At temperatures below the static Leidenfrost point TL, the transition from deposition to splash is followed by another disappearance of splashing, before it reappears at larger impact velocity in a wide range of parameters. Above TL, splashing occurs at tremendously reduced impact velocity. We analyse this peculiar behaviour using different high speed imaging techniques.

CPP 47.8 Wed 17:00 H3

Morphology of liquid-liquid dewetting — •Roghayeh Shiri[1], Ralf Seemann[1], Dirk Peschka[2], and Barbara Wagner[2] — [1]University of Saarland, Saarbrucken, Germany — [2]Weierstrass Institute, Berlin, Germany.

We study the spinodal dewetting of nanometric thin liquid polystyrene (PS) films on liquid polymethyl-methacrylate (PMMA) substrates. The initial stage of dewetting consists of the amplification of thermal fluctuations driven by dispersion forces, eventually leading to the formation of holes with a preferred distance λ. According to theoretical predictions, the PS/air and the PS/PMMA interfaces shall evolve in a coupled way. As the surface tension of the PS/PMMA interface is way smaller than the surface tension of the PS/air interface, the amplitude of the corrugation of the PS/PMMA interface will be much larger than that of the PS/air interface. To determine the morphological evolution of the preferred wavelength λ and of the preferred holes distance, we follow the evolution of PS/air interface in situ by atomic force microscopy (AFM). The evolution of the PS/PMMA interface is explored ex situ by AFM using a lift up technique. By matching the PS/air and the PS/PMMA interfaces we can decide if the coupled corrugations of both interfaces evolve in phase or anti phase. We also explore the dependence of the preferred wavelength as function of PS film thickness and compare the result with theoretical predictions.

15 min. break

CPP 47.9 Wed 17:30 H3

Multiparticle Collision Dynamics Modeling of Nematic Liquid Crystal with Variable Order Parameter — •Shubhadeep Mandal[1] and Marco G. Mazza[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Loughborough University, Loughborough, United Kingdom

We have generalized the particle-based multiparticle collision dynamics (MPCD) method to model the hydrodynamics of nematic liquid crystals. Following Qian-Sheng theory [Phys. Rev. E 58, 7475 (1998)] of nematic liquid crystals, the spatial and temporal variations of the nematic director field and the nematic degree of order are described by a tensor order parameter. The principle idea is to assign a tensor quantity to each MPCD particle, whose average resembles the macroscopic tensor order parameter. The applicability of this new method is verified by performing several physical and numerical tests. We have tested: (a) the isotropic-nematic phase transition, (b) the annihilation dynamics of a pair of point defects, (c) the flow alignment of the nematic director in shear and Poiseuille flows, and (d) the velocity profile in shear and Poiseuille flows. We have found excellent agreement with existing literature. Additionally, we study the decay of force-dipole flow field in nematic liquid crystals. The present method can have far-reaching implications not only in modeling of nematic flows, but also to study the motion of colloids and microswimmers immersed in an anisotropic medium.

CPP 47.10 Wed 17:45 H3

Kinetic Monte Carlo simulations of thin film growth for pure and mixed films — •Eelco Empting, Miriam Klopotek, and Martin Oettel — Institut für angewandte Physik, Tübingen, Germany

We consider a binary lattice model for growth of demixing thin films, i.e. where two species of particles are deposited onto a substrate and undergo diffusion at and above it. Particle interactions include hard-core repulsion and nearest-neighbor attraction, the strength of which depends on the species of the particles involved. In KMC simulations of this model, we consider quite generally all sorts of single particle moves to neighboring sites, thus allowing for species-dependent diffusion constants, desorption, and formation of cavities.

We studied the influence of the various parameters, most notably diffusion rates and interaction strengths, on the structure and evolution of a growing film. Among other things, this system was used to compare simulations to real-world growth experiments of a C60-CuPC blend film where we can identify the defining parameters leading to characteristic structure in the films.

CPP 47.11 Wed 18:00 H3

Classical density functional theory for ferrogels with distinguishable particles — •Segun Goh, Andreas M. Menzel, and Hartmut Löwen — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany

Classical density functional theory has been widely studied for liquid-like states of materials which consist of indistinguishable particles interacting via pairwise potentials. Meanwhile, there are materials, among which ferrogels provide one of the important examples, where the particles are fixed in an elastic polymer matrix. As particle neighbors do not change over time due to the fixation, particles are distinguishable by positions in those systems. In this talk, we discuss a density functional approach for such systems with distinguishable particles, considering a two-dimensional bead-spring lattice with magnetic dipoles at every bead as a model for ferrogels. We first introduce a mapping of the harmonic springs representing the elastic matrix onto a pairwise pseudo-interaction between indistinguishable particles. The mapping is justified by Monte-Carlo simulations of both the bead-spring model and the frozen states of corresponding pseudo-interaction systems in combination with the density functional theory. We then formulate density functional theory for the dipole-spring model and investigate magnetostriction and compression moduli of ferrogels under magnetic interactions. We expect that our density functional approach may provide a route towards an understanding of a broad range of materials with particle inclusions.

CPP 47.12 Wed 18:15 H3

Crystallization of spheres with static and dynamic size dispersity — •Praveen Kumar Bommineni, Nydia Roxana Varela Rosales, Marco Klement, and Michael Engel — Institute for Multiscale Simulation, Friedrich-Alexander University Erlangen-Nürnberg, Nägelsbachstrasse 49b, 91052 Erlangen, Germany

Colloids are rarely uniform but follow a distribution of sizes, shapes, and charges. This dispersity can be inherent (static) or develop and change over time (dynamic). Despite a long history of research, the conditions under which non-uniform particles crystallize and which crystal forms is still not well understood. Here, we demonstrate that hard spheres with Gaussian radius distribution and dispersity up to 19% always crystallize if compressed slow enough, and they do so in surprisingly complex ways [1]. This result is obtained by accelerating event-driven simulations with particle swap moves for static dispersity and particle resize moves for dynamic dispersity. Above 6% dispersity, AB_2 Laves, AB_{13}, and a region of complex Frank-Kasper phases are found. The Frank-Kasper region includes a quasicrystal approximant with Pearson symbol oS276. Our findings are relevant for ordering phenomena in soft matter and alloys.

[1] P.K. Bommineni et al., arXiv:1811.00061.

CPP 47.13 Wed 18:30 H3

Elastic turbulence at low Reynolds numbers and its control — •Reinier van Buel, Christian Schaaf, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

The properties of viscoelastic solutions are exceptionally applicable on the micron scale. For example, in microfluidic devices mixing and heat transfer are strongly enhanced. This is due to elastic turbulence [1], which bears similar qualities as inertial turbulence. The relevant dimensionless number characterizing viscoelastic fluids is the Weissenberg number, which compares the polymer relaxation time to the characteristic time of the flow dynamics.

Numerical solutions of the Oldroyd-B model in a two-dimensional Taylor-Couette geometry display a supercritical transition from the laminar Taylor-Couette to the occurence of a secondary flow [2]. The secondary flow is turbulent and caused by an elastic instability beyond a critical Weissenberg number. The order parameter, the time average of the secondary-flow strength, follows the scaling law $\Phi \propto (\mathrm{Wi}-\mathrm{Wi}_c)^\gamma$ with $\mathrm{Wi}_c = 10$ and $\gamma = 0.45$ and the power spectrum of the velocity fluctuations shows a power-law decay with a characteristic exponent. Finally, we present first results on controlling the elastic instability through an oscillating rotation of the outer cylinder of the Taylor-Couette cell, with a frequency close to the characteristic relaxation time of the dissolved polymers.

[1] A. Groisman and V. Steinberg, Nature **405**, 53 (2000).

[2] R. Buel, C. Schaaf, H. Stark, Europhys. Lett. **124**, 14001 (2018).

CPP 47.14 Wed 18:45 H3

Gold nanoclusters at room temperature: are they soft matter? — •Luca M. Ghiringhelli, Bryan Goldsmith, Diego Guedes-Sobrinho, Jacob Florian, Jin-Xun Liu, Weiqi Wang, Juarez Da Silva, Ian Hamilton, and Matthias Scheffler — Fritz-Haber- Institut der Max-Planck-Gesellschaft, Berlin, Germany

Soft matter encompasses systems for which the predominant physical behaviors occur at an energy scale comparable with room-temperature (T=300 K) thermal energy. Here, we present a study of free-energy landscapes of neutral gold nanoclusters in the size ranges 10–13 (arXiv:1811.08062) and 25–40 (arXiv:1811.04438) atoms. Gold nanoclusters are interesting for their possible applications in gas sensing, pollution reduction, and catalysis. Our studies are based on extensive Born-Oppenheimer density-functional-theory replica-exchange molecular-dynamics sampling over a wide range of temperatures. We find that the long-standing question “At which *size* (neutral) gold clusters start favoring 3D vs 2D structures?” should be recast, at least in the size range between 10 and 13 atoms, into the question (here answered): “At which *temperatures* are 3D structures favored?”. At T=300 K, we find that the typical activation barrier of Au–Au bonds is indeed comparable with the thermal energy, resulting in a continuous reshuffling of bonds and, in the size range 25–40 atoms, in low free-energy structures that significantly differ from the T=0 K structures. In these examples, gold nanoclusters seem indeed to match the definition of soft matter. This might have important implications for the characterization of the chemical reactivity of these systems.

CPP 47.15 Wed 19:00 H3

MIEZE spectroscopy of sub-picosecond collective dynamics in bulk liquid water — Olaf Soltwedel[1,2], •Leonie Spitz[3], Johanna K Jochum[3,4], Andreas Wendl[1], Christian Pfleiderer[1], and Christian Franz[3] — [1]Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany — [2]Technische Universität Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt, Germany — [3]Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany — [4]Bayerisches Geoinstitut, Universität Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany

The anomalously large dielectric constant of water is intimately connected with a Debye relaxation peak in low frequency dielectric spectra. Despite intense research, a link between the molecular dynamics and the Debye relaxation peak, are still under heavy debate. Proposed mechanisms include translational and/or rotational motions, movement of free water molecules, collective relaxation of a cluster or hopping of defects in the hydrogen bond network. We used MIEZE (Modulation IntEnsity with Zero Effort) neutron spin echo spectroscopy, a high resolution time of flight technique, to measure the dynamic structure factor (S(q,t)) of water over an exceptional dynamical range (0.01 up to 1000ps). Consistent with the literature, we find the bulk transverse diffusion on length scales from 0.1/Å up to 0.4/Å. As our main result, reveals at least two more processes on sub-picosecond time-scales. This provides direct evidence of a vibration and/or delocalization of hydrogen larger than the intermolecular distance as proposed [1].

[1] A. Arbe et al. PRL 117, 185501 (2016)

CPP 48: Biopolymers, Biomaterials and Bioinspired Functional Materials (joint session CPP/BP)

Time: Wednesday 15:45–18:30 Location: H13

Invited Talk CPP 48.1 Wed 15:45 H13

Many Weak Interactions Make a Difference - from Fuzzy Biomolecular Self Assembly to Superselectivity — •Ralf Richter — School of Biomedical Sciences, Faculty of Biological Sciences, School of Physics and Astronomy, Faculty of Mathematics and Physical Sciences, and Astbury Centre for Structural Molecular Biology, University of Leeds, Leeds, LS2 9JT, United Kingdom

Multivalent interactions are key to molecular and cellular communication in biological systems, yet remain poorly understood. I shall present results of our efforts to better understand the role of multivalent interactions in two biological systems that involve biological polymers: (i) the nuclear pore permeability barrier, a meshwork of intrinsically disordered proteins that fills the nuclear pores and makes nucleo-cytoplasmic transport selective, and (ii) the interface between polysaccharide-rich extracellular matrix and the cell surface which is key to the communication of cells with their environment.

To study these systems on the supramolecular level, we take a multidisciplinary approach that combines surface science tools (to reconstitute well-defined model systems from the constituent molecules), biophysical characterization techniques (for quantitative analysis) and soft matter physics theory (to establish structure/property/function relationships).

The insights gained help us to uncover physical mechanisms underpinning functions, such as 'superselectivity' in the targeting of cell surfaces or the permeability of membranes, and help develop materials with new functions for applications in the life sciences.

CPP 48.2 Wed 16:15 H13

DNA crookedness regulates DNA mechanical properties at short length scales — •J.G. Vilhena[1], Alberto Marin-Gonzalez[2], Fernando Moreno-Herrero[2], and Ruben Perez[3] — [1]Department of Physics, University of Basel — [2]Centro Nacional de Biotecnologia, CSIC, Spain — [3]Universidad Autonoma de Madrid, Spain

Sequence-dependent DNA conformation and flexibility play a fundamental role in specificity of DNA-protein interactions. Here we quantify the DNA crookedness: a sequence-dependent deformation of DNA that consists on periodic bends of the base pair centers chain. Using extensive 100 μs-long all-atom molecular dynamics simulations, we found that DNA crookedness and its associated flexibility are bijective: unveiling a one-to-one relation between DNA structure and dynamics. This allowed us to build a predictive model to compute the stretch moduli of different DNA sequences from solely their structure. Sequences with very little crookedness show extremely high stretching stiffness and have been previously shown to form unstable nucleosomes and promote gene expression. Interestingly, the crookedness can be tailored by epigenetic modifications, known to affect gene expression. Our results rationalize the idea that the DNA sequence is not only a chemical code, but also a physical one that allows to finely regulate its mechanical properties and, possibly, its 3D arrangement inside the cell.

CPP 48.3 Wed 16:30 H13

Fast and on demand mussle-inspired adhesives by enzymatic polymerization of decapetides — •Maximilian Seuss[1], Justus Horsch[2], Patrick Wilke[2], Matthias Pretzler[3], Inga Melnyk[1], Dario Remmler[2], Annette Rompel[3], Hans G. Börner[2], and Andreas Fery[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V. — [2]Humboldt-Universität Berlin — [3]Universität Wien

A novel strategy to generate adhesive protein analogues by enzyme-induced polymerization of peptides is presented. Inspired by the repetitive nature of certain peptide sequences in mussel-foot protein mfp-1 we designed a polymerization reaction using these sequences as macromonomers. Peptide polymerization relies on tyrosinase oxidation of tyrosine residues to Dopaquinone, which rapidly forms cysteinyldopa with free thiols from cysteine residues. This forms a covalent bond between macromonomers and generates adhesive polymers. The resulting artificial protein analogues show strong adsorption to different surfaces, even resisting hypersaline conditions. Adhesion energies up to 10.9 mJ/m^2 are found in single adhesion events and average values are superior to those reported for mussel foot proteins that constitute the gluing interfaces.

CPP 48.4 Wed 16:45 H13

Inequivalence of fixed-force and fixed-extension statistical ensembles for a flexible polymer tethered to a planar substrate — •Panayotis Benetatos[1] and Sandipan Dutta[2] — [1]Department of Physics, Kyungpook National University, Daegu, S. Korea — [2]Center for Soft and Living Matter, Institute for Basic Science, Ulsan, S. Korea

Recent advances in single macromolecule experiments have sparked interest in the ensemble dependence of force-extension relations (Gibbs versus Helmholtz). The thermodynamic limit may not be attainable for such small systems, that leads to inequivalence of the fixed-force and the fixed-extension ensemble. We consider an ideal Gaussian chain described by the Edwards Hamiltonian with one end tethered to a rigid planar substrate. We analytically calculate the force-extension relation in the two ensembles and we show their inequivalence which is caused by the confinement of the polymer to half space. The inequivalence is quite remarkable for strong compressional forces. We also perform Monte-Carlo simulations of a tethered wormlike chain with contour length 20 times its persistence length which corresponds to experiments measuring the conformations of DNA tethered to a wall. The simulations confirm the ensemble inequivalence and qualitatively agree with our analytical predictions for the Gaussian model. Our analysis shows that spatial confinement due to tethering causes ensemble inequivalence, irrespective of the polymer model.

15 min. break

CPP 48.5 Wed 17:15 H13

Transverse viscoelastic properties of cellulose fibers investigated by atomic force microscopy — •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 of Paper, Pulp and Fibre Technology, Graz University of Technology, Austria — [3]CD Laboratory for Fiber Swelling and Paper Performance, Graz University of Technology, Austria

Cellulosic fibers are used in the paper and textile industry. To gain more insight on how mechanical properties of cellulose fibers are related to properties of end-products like paper, our work focusses on the transverse viscoelastic behavior of single cellulose fibers. To reach this ambitious goal we implemented an atomic force microscopy (AFM) based method. Probing nanoscale mechanical properties of soft materials with AFM yields information on the performance of the material. With the Johnson-Kendall-Roberts model, the contact between AFM tip and sample surface can be well described. The evaluation of the experimental data combines contact mechanics and viscoelastic models which consist of springs and dashpots in series or parallel describing elastic and viscous behavior, respectively. Here, it will be demonstrated that the so-called Generalized Maxwell model yields reasonable results for single pulp as well as viscose fibers at five different relative humidity (RH) values and in water. The RH increase leads to a steady decrease of the viscoelastic properties. Especially in water, the viscoelastic behavior shows a pronounced decrease, proving that the interaction of the fibers in water is different than at varying RH levels.

CPP 48.6 Wed 17:30 H13

Elastic-Plastic Transition of Filament Networks — •Fanlong Meng[1] and Eugene Terentjev[2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]Cavendish Laboratory, University of Cambridge, JJ Thomson Avenue, Cambridge CB3 0HE, U.K.

Filament networks are ubiquitous in biological systems, such as cytoskeleton, extracellular matrix and connective tissue. The elasticity of a permanently crosslinked filament network is relatively well understood [1, 2]. However, the filament networks are usually transient because the filaments can dynamically break from and re-bonded to crosslinks including various proteins and biological motors. Because of the complexity in the spatial and the temporal evolution of the network structure induced by crosslink dynamics, the rheological properties of a transiently crosslinked is poorly investigated. Recently, we proposed a model where the total energy of a transient filament network is a function of time due to the breakage and the re-formation of crosslinks [3]. With the model, we successfully explain experimental observations including stress relaxation, shape recovery, and necking formation. Moreover, we provide a phase diagram detailing the conditions for a transient filament network to behave elastically, plastically or in a mixed way. References: [1] F. Meng, E. Terentjev, Soft Matter 12, 6749 (2016) [2] F. Meng, E. Terentjev Polymers, 9, 52 (2017) [3] F. Meng, E. Terentjev, Macromolecules 51, 4660 (2018)

CPP 48.7 Wed 17:45 H13

Permanent Damage in Reversible Cross-linked Fiber Bundles — •Huzaifa Shabbir[1] and Markus Hartmann[2] — [1]Faculty of Physics, University of Vienna, Austria — [2]Ludwig Boltzmann Institute of Osteology at the Hanusch Hospital of WGKK and AUVA Trauma Centre Meidling, Vienna, Austria

Cross-linking is a common strategy to tailor the mechanical properties of polymeric systems. In natural systems, these cross-links are usually weaker than covalent bonds, which helps to maintain the structural integrity of the system preventing permanent damage [1].

Addition of cross-links to a polymeric system shows positive effects on many mechanical parameters, recent computational studies on cross-linked fiber bundles showed the surprising result that weak cross-links may deteriorate the strength of these systems [2]. This effect is strongly dependent on the coordination of cross-links [3], being most pronounced for the classical case of two-fold coordinated cross-links, i.e. one additional bond connecting two monomers. This presentation will discuss in detail the influence of cross-link coordination on this effect. In particular, Monte Carlo simulations have been used to detect the onset of permanent damage, the corresponding work and strength as a function of cross-link density and coordination. The results clearly indicate that systems with cross-links of higher coordination are more damage tolerant than classical two-fold coordinated cross-links.

[1] Fantner et al., Biophys. J. 90, 1411 (2006) [2] Nabavi & Hartmann, Soft Matter 12, 2047 (2016) [3] Shabbir & Hartmann, New Journal of Physics 19, (2017)

CPP 48.8 Wed 18:00 H13

Capabilities of photoresists based on polysaccharides for Direct LaserWriting — •Marie-Christin Heep[1], Agnes Koerfer[1], Maximilian Rothammer[2], Cordt Zollfrank[2], and Georg von Freymann[1,3] — [1]Physics Department and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]Chair of Biogenic Polymers, TU Munich, Campus Straubing of Biotechnology and Sustainability, Germany — [3]Institute for Industrial Mathematics ITWM, Germany

Direct laser writing is a common method for fabrication of three dimensional micro- and nanostructures. The available materials have recently been expanded to polysaccharides [1]. These resists consist of a photo-curable polysaccharide, a photo initiator and a solvent. The exact mixture defines the properties of the final material. A detailed discussion on the crosslinking density and hence the stability of the written structures as well as on the resolution and the feature size of the resist will be provided. These properties are most crucial for applications. Furthermore, we examine the surface roughness of the resist as well as the ability to self-assemble. The self-assembling of the resist is investigated with respect to the concentration of initiator. Different solvents are taken into account, to observe their influence on the handling of the resist. The knowledge about the influence of the exact mixture on the properties of the material allows the development of new resist for specific requierenments. This also allows the use of self-assembling processes for micro- and nanostructures with a tailored disorder.

[1] M. Rothammer et al., Cellulose **25**, 6031 (2018).

CPP 48.9 Wed 18:15 H13

Towards an artificial human nail plate — •Kim Thomann[1], Andreas Späth[1], and Rainer H. Fink[1,2] — [1]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]CENEM, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

Human fingernails cannot be studied ex vivo with the same ease as for example hair since only clippings can be obtained which do not necessarily reflect the behavior of the whole nail. Thus, we aim to create an artificial nail plate model that resembles the adhesive characteristics of the human finger nail suited for ex vivo studies. In order to mimic the surface free energy (SFE) as well as the morphology of the nail, we first investigated the surface properties of the natural fingernail using a number of methods. In vivo contact angle (CA) measurements were performed to determine the SFE. Water CAs along resin replicas of fingernails were measured and scanning electron micrographs were taken to correlate SFE with topography. Our first approach for an artificial nail plate model is based on mixed alkane thiol self-assembled monolayers, terminated with either -OH or -COOH and -CH3. CA measurements revealed that either the total SFE or the relation between the polar and dispersive component could be replicated, but both requirements could not be met simultaneously. Thus, micro-contact printing (micro-CP) is considered to produce patterned SAMs at various periods to match the nail's microstructure.

CPP 49: Hydrogel und Microgel

Time: Wednesday 17:15–18:30 Location: H18

Invited Talk CPP 49.1 Wed 17:15 H18

Stimuli-Responsive Polymer-Based Sensors, Muscles, and Drug Delivery Platforms — •Michael Serpe — University of Alberta, Edmonton, AB, Canada

The group's research is focused on the development of novel polymer-based materials for solving environmental and health-related problems. To solve these problems, the group primarily employs poly (N-isopropylacrylamide) (pNIPAm)-based spherical particles as the active component in our technologies. PNIPAm-based particles (nano or microgels, depending on their diameter) are extremely porous, and are fully water soluble and swellable. Additionally, pNIPAm-based nano/microgels are responsive to temperature, shrinking in diameter as the temperature is increased to >32 °C and reswelling when they are cooled to < 32 °C. Our group has exploited these properties for numerous applications. Today's talk will highlight the group's work on the development of these devices for sensing and biosensing, as muscles, and for controlled/triggered drug delivery.

CPP 49.2 Wed 17:45 H18

Multiresponsive PNIPAM Microgels Doped with Magnetic Nanoparticles — •Marcus U. Witt[1], Nadir Möller[1], Melissa Hess[2], Stephan Hinrichs[3], Birgit Fischer[3], Anette Schmidt[2], and Regine v. Klitzing[1] — [1]Technische Universität Darmstadt, Institut für Festkörperphysik, Alarich-Weiss-Straße 10, 64287 Darmstadt — [2]Universität zu Köln, Institut für Physikalische Chemie, Luxemburger Straße 116, 50939 Köln — [3]Universität Hamburg, Institut für Physikalische Chemie, Grindelallee 117, 20146 Hamburg

Microgels based upon N-isopropylacrylamide (NIPAM) exhibit a volume phase transition at a temperature of 32°C (VPTT) in water. Several additives can be used to tailor physical and chemical properties. Co-monomers are incorporated to induce a response mechanism to pH or ionic strength. Non-organic particles can be loaded into the microgel to add a response to external stimuli such as light and magnetic fields. The present study addresses microgels with different inner structures (heterogeneous, homogeneous, *onion-like*) loaded with magnetic nanoparticles (MNP) leading to different MNP distribution. The effect of MNP loading on the VPTT is studied by light scattering and zeta potential measurements. The response of those ferrogels to external magnetic fields is investigated in bulk and at the surface. Magneto-relaxation measurements show unexpected and counterintuitive results, leading to the conclusion that the MNP rearrange while crossing the VPTT.

CPP 49.3 Wed 18:00 H18

Incorporation of conductive materials in stimuli-responsive hydrogel films synthetized by ionizing radiation for the development of biomedical sensor applications — •Jesus Eduardo Lopez-Barriguete[1,2], Gabriel Flores-Rojas[1,2], Felipe Lopez-Saucedo[1], Takashi Isoshima[2], and Emilio Bucio[1] — [1]Departamento de Química de Radiaciones y Radioquímica, Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, Circuito exterior, Ciudad Universitaria, Ciudad de México 04510, México — [2]Nano Medical Engineering Laboratory, RIKEN, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan

Stimuli-responsive systems of co-polymeric hydrogels with a specific temperature (38 and 39 *C) response has been prepared and modified to elaborate adaptable films for biomedical and nanotechnology applications. The principal thermo-responsive polymer is N-isopropyl acrylamide (PNIPAAm) with the addition of dimethyl acrylamide (DMAAm) for temperature modification, methyl methacrylate (MMA), and ethoxyethyl methacrylate (EEM) for mechanical improvements. Ionizing radiation technique (gamma rays) allows synthesizing different systems at a dose radiation of 50 kGy. The matrix modification with silver and copper incorporation was by chemical synthesis. The conductive properties of these materials and biocompatibility could permit the addition of electrical properties to the films admitting electrical changes by the internal structure variation of the polymeric chains due to the temperature variability. All the samples were characterized by FT-IR, DSC, SEM, and EDX.

CPP 49.4 Wed 18:15 H18

Non-additive ion effects on polymer coil-globule collapse transitions in mixed salt solutions — •Nico van der Vegt[1], Ellen E. Bruce[1], Pho T. Bui[2], Bradley A. Rogers[2], and Paul S. Cremer[2] — [1]Technische Universität Darmstadt, Germany — [2]Pennsylvania State University, USA

Non-additive ion effects in Hofmeister ion chemistry impact properties of aqueous soft matter but are poorly understood to date. I will present ion-specific effects on the lower critical solution temperature of poly(N-isopropylacrylamide) in mixed electrolyte solutions. Significantly, I will show that polymer hydration and polymer-anion interactions can be regulated in the presence of weakly (NaI) and strongly hydrated (Na2SO4) mixed salts, leading to both collapse and swelling of the polymer. The underlying mechanisms are discussed based on insights obtained from computer simulations and vibrational sum frequency spectroscopy (VSFG) experiments.

CPP 50: Organic Electronics and Photovoltaics III - Organic Photovoltaics

Time: Thursday 9:30–13:00 Location: H18

CPP 50.1 Thu 9:30 H18

Achieving supressed recombination; kinetics of singlet and triplet charge transfer states defining charge generation and recombination in organic solar cells — •Safa Shoai — University of Potsdam

In-depth understanding of charge carrier photogeneration and recombination mechanism in organic solar cells is still an ongoing effort in the community. In donor:acceptor (bulk) heterojunction organic solar cells charge photogeneration and recombination are inter-related via the kinetics of charge transfer states. While efficient charge photogeneration quantum yield can be achieved in many donor:acceptor systems, only very few systems have so far shown significantly reduced bimolecular recombination coefficient. Herein, we present a meta-analysis of the device performance for numerous BHJ OSC for which field dependent photogeneration, charge carrier mobility and fill factor are determined. From this analysis we find a spin-related factor which is dependent on the ratio of back electron transfer of the triplet CT states to the decay rate of the singlet CT states. This factor along with the dissociation efficiency of the CT states primarily define the charge generation efficiency and bimolecular recombination reduction factor. In systems with extremely efficient charge generation due to the very fast dissociation rate of the CT states, the recombination can be strongly suppressed regardless of the spin-related factor.

CPP 50.2 Thu 9:45 H18

The charge transfer state in organic solar cells: contribution of static disorder and molecular reorganisation — •Clemens Göhler and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Solar cells from organic semiconductors use an active layer consisting of a heterogeneous blend of electron acceptor and donor materials, such as fullerenes and conjugated polymers. The donor HOMO and acceptor LUMO level in these heterojunctions form an additional charge transfer (CT) state, which can be detected with electro-optical spectroscopy methods.

Molecular properties of donor copolymers, such as molecular weight, defects, or stoichiometry, are crucial to the solar cells performance - predominantly by affecting short circuit current and fill factor. Their impact upon the open circuit voltage, which is connected to the CT states energy, might not be as distinct. They are, however, affecting the CT states energetic distribution, which can be described as a convolution of its molecular reorganisation energy and the amount of energetic disorder. We are able to unravel both contributions using temperature dependent sub-gap photocurrent spectroscopy to contribute to a deeper understanding of the CT states role in solar cell performance.

CPP 50.3 Thu 10:00 H18

Evaluation of molecular donor-acceptor pairs forming charge-transfer or exciplex states — •Thomas Zechel, Thomas Schröther, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86159 Augsburg

Intermolecular excited states play a major role in various organic semiconductor applications. Charge-transfer (CT) states were shown to be a major contributor to large voltage losses in organic photovoltaic cells (OPVCs) and exciplex systems are becoming a viable alternative to heavy metal complexes in organic light emitting diodes (OLEDs). Both states are formed by at least two molecules of different kind (acceptor and donor). In both cases for the excited state the hole of the bound exciton resides on the donor and the electron resides on the acceptor molecule. The difference between the two being that the exciplex only exists in the excited state (no direct ground state absorption) while the CT state exhibits a small but measurable direct absorption from the ground state. This main difference is accompanied by considerably larger external electroluminescent quantum yields ($\mathrm{EQE_{EL}}$) for exciplex systems compared to CT systems.

In this work a number of different donor-acceptor pairs which usually form exciplexes or CT states are investigated using electrical (current-voltage-luminescence, incident photon to current efficiency), optical (EL, PL) and computational (density functional theory simulations) methods to gain further insights into the differences and similarities of CT and exciplex systems on a basic material level.

CPP 50.4 Thu 10:15 H18

Exciton Dynamics in Pentacene-Perfluoropentacene Heterostructures — •Vipilan Sivanesan[1], Frank Schreiber[2], Katharina Broch[2], and Petra Tegeder[1] — [1]Universität Heidelberg, Physikalisch-Chemisches Institut — [2]Universität Tübingen, Institut für Angewandte Physik

Understanding the ultrafast electronically excited state dynamics in organic semiconductors after optical excitation is crucial for the optimization of organic optoelectronic devices. Moreover, the knowledge of the morphology and energetics at donor-acceptor interfaces is important for efficient charge separation in organic solar cells. Thereby, charge transfer (CT) states play a decisive role. To analyse the ultrafast processes at the interface more precisely, both well-defined structures of the samples and a very high time resolution in the experiment are required. In this work we investigated thin films of pentacene (PEN), perfluoropentacene (PFP), and various heterostructures of PEN and PFP by means of femtosecond time-resolved second harmonic generation. For the donor/acceptor configurations, depending on the molecular orientations at the interface and the excitation energies, the dynamics of CT-states were analyzed.

CPP 50.5 Thu 10:30 H18

Impact of Structural Defects on the Energy Level Alignment in planar Pentacene-Perfluoropentacene Heterojunctions — •Jan Hagenlocher[1], Alexander Hinderhofer[1], Satoshi Kera[2], and Frank Schreiber[1] — [1]Universität Tübingen, Tübingen, Germany — [2]Institute for Molecular Science, Okazaki, Japan

The majority of today's organic (opto-)electronic devices comprise a number of different organic-semiconductor layers. The functionality of such complex heterostructures depends on the relative alignment of the frontier molecular-orbital energies in the individual layers with respect to those in all others. In this study we investigated the dependence of this energy level alignment on structural defects in an organic-organic heterojunction of perfluoropentacene (PFP)-on-pentacene (PEN) using x-ray scattering, atomic force microscopy and ultraviolet photoelectron spectroscopy. The density of structural defects was varied by changing the growth temperature of the bottom PEN film. A direct relationship between the defect density and the energy level alignment was found, where the binding energies together with a change in the electrostatic potential at the interface vary systematically with the defect density. This indicates that a key factor affecting the energy level alignment is the number of transferred electrons from the substrate to unoccupied gap states in the PFP film. The described gap states originate from the structural defects and can be effectively controlled by adjusting the growth conditions of the organic films.

CPP 50.6 Thu 10:45 H18

Microscopic effects of the broadening of the density of states in donor-acceptor blends and their role in organic photovoltaics — •Michel Panhans[1], Sebastian Hutsch[1], Johannes Bednuhn[2], Karl Sebastian Schellhammer[1], Koen Vandewal[3], and Frank Ortmann[1] — [1]Center for Advancing Elec- tronics Dresden, TU Dresden — [2]Institut für Angewandte Physik, TU Dresden — [3]Institute for Materials Research (IMO-IMOMEC), Hasselt University, Wetenschapspark 1, 3590 Diepenbeek, Belgium

Microscopic understanding and quantifying the density of states including linewidth broadening and dissipation mechanisms in organic semiconductors [1,2] plays a crucial role for designing efficient solar cells and transistors. We study models of fullerene based donor-acceptor systems regarding their response to optical excitations. We analyze the density of states (DOS) and excited-state DOS with electronic disorder and electron-phonon interaction based on ab initio simulations. The calculated temperature dependence of the absorption linewidth is compared to temperature dependent absorption measurements on the same blends where we find very good agreement. Finally, we discuss implications for the open-circuit voltage in organic solar cells.

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

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

CPP 50.7 Thu 11:00 H18

Energy Distribution of Charge-Transfer Excitons at Organic Donor-Acceptor Interfaces: Simulations for Room Temperature — •Sebastian Schellhammer[1,2], Gianaurelio Cuniberti[1,2], and Frank Ortmann[2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Technische Universität Dresden, 01062 Dresden, Germany — [2]Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany

Charge transfer (CT) excitons at donor-acceptor interfaces determine the performance of organic solar cells. The subgap absorption by such excitons is also used to design sensitive near-infrared photodetectors based on the broad CT exciton bands. However, the prediction of the energetics of the CT exciton band has ever been a great challenge. We present an approach for an efficient computation of the CT energies at room temperature based on time-dependent density functional theory including the band tail broadening induced by thermal fluctuations in a semi-classical way. This method is demonstrated for different donor molecules with C60 as electron accepting material. A comparison to experimental CT band characteristics shows excellent agreement for both the linewidth broadening as well as the CT energies. The approach thus combines accuracy with modest computational cost.

15 min. break

CPP 50.8 Thu 11:30 H18

How to Interpret Absorption and Fluorescence Spectra of Charge Transfer States in an Organic Solar Cell — •Frank-Julian Kahle[1], Alexander Rudnick[1], Heinz Bässler[2], and Anna Köhler[1,2] — [1]Soft Matter Optoelectronics, Department of Physics, University of Bayreuth, Germany — [2]Bayreuth Institute of Macromolecular Science (BIMF), University of Bayreuth, Germany

The aim of the present work is to identify the appropriate framework for analyzing photoluminescence and photocurrent (EQE) spectra of charge transfer (CT) states in donor-acceptor blends used as active materials for organic solar cells. We applied gated photoluminescence (PL) spectroscopy within a temperature range from 5 to 295 K combined with EQE as well as electroluminescence (EL) experiments on 1:1 Me-LPPP:PCBM blends by weight. We find that the PL spectra are virtually temperature independent and the temporal decay of the emission features a power law with an exponent close to -3/2 as Hong and Noolandi predicted for distributed geminately bound electron-holes pairs. The results are inconsistent with both Marcus* electron transfer theory and the original Marcus-Levich-Jortner (MLJ) theory, and they prove that disorder effects are crucial. Both PL and EQE spectra can be rationalized in terms of the classic Franck-Condon picture of electronic transitions that couple to intra-molecular vibrations as well as low frequency modes of the donor-acceptor pair that forms the CT state.

CPP 50.9 Thu 11:45 H18

Absence of charge transfer state enables very low VOC losses in SWCNT:fullerene solar cells — •Andrej Classen[1], Lukas Einsiedler[1], Thomas Heumüller[1], Arko Graf[2], Maximilian Brohmann[2], Felix Berger[2], Simon Kahmann[1], Moses Richter[1], Gebhard Matt[1], Karen Forberich[1], Jana Zaumseil[2], and Christoph Brabec[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Ruprecht-Karls-Universität Heidelberg

Current state of the art organic solar cells (OSC) still suffer from high losses of open circuit voltage (VOC). Conventional polymer:fullerene solar cells usually exhibit band gap to VOC losses greater than 0.8 V. Here a detailed investigation of VOC is presented for solution processed OSCs based on (6,5) single-walled carbon nanotubes (SWCNT):[6,6]-phenyl-C71-butyric acid methyl ester (PC70BM) active layers [1]. Considering the very small optical band gap of only 1.22 eV of (6,5) SWCNTs, a high VOC of 0.59 V leading to a low Egap/q - VOC = 0.63 V loss is observed. The low voltage losses are partly due to the lack of a measurable charge transfer state and partly due to the narrow absorption edge of SWCNTs. Consequently, VOC losses attributed to a broadening of the band edge are very small resulting in VOC,SQ - VOC,rad = 0.12 V. Interestingly, this loss is mainly caused by minor amounts of SWCNTs with smaller band gaps as well as (6,5) SWCNT trions. More intriguingly, we find a very low voltage loss due to nonradiative recombination, ΔVOC,nonrad = 0.26 V, which is exceptional for fullerene based OSCs.

[1] Classen et al., Adv. Energy Mater., 2018, 1801913

CPP 50.10 Thu 12:00 H18

Investigating in-operando the effects of solvent additives on the stability of organic solar cells based on PTB7-Th:PC71BM — •Dan Yang[1], Franziska 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

Due to low cost, flexibility, solution processing and large-scale fabrication, enormous attention is focusing on the research and development for higher organic photovoltaics performance over the last decades. In recent years, the power conversion efficiency (PCE) of organic solar cells(OSCs) of single-junction OSCs has reached 14.6 %, which is still lower than the inorganic counterparts. To further optimize the performance, additive solvents are widely used in the solution of bulk heterojunction. While the influents of those additives on the device degradation behavior are essential to be disclosed. In this work, PTB7-Th: PC71BM solar cells with two different additive solvents are probed with in-operando GISAXS measurements to resolve the morphology changes during operation. Combining with the J-V performance, the degradation mechanisms behind the additive solvents is figured out.

CPP 50.11 Thu 12:15 H18

Toward a universal polymeric material for electrode buffer layers in organic and perovskite solar cells and organic light-emitting diodes — Qiang Zhang[1], Wei-Ting Wang[2], Tobias Wächter[3], •Michael Zharnikov[3], Yian Tai[2], and Der-Jang Liaw[1] — [1]Polymer Science and Materials Lab., Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei 10607, Taiwan — [2]Nanohybrid Materials and Devices Lab., Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei 10607, Taiwan — [3]Applied Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany

A novel concept of a "universal" electrode buffer layer material, exhibiting either hole transporting or reducing electrode work function properties, is demonstrated by the example of a polymeric compound PDTON. Depending on the composition ratio of acetic acid and ethyl acetate upon dispersing, PDTON forms two kinds of nanospheres, serving as building blocks and defining the properties of the respective materials, termed as A-PDTON and C-PDTON. These materials are suitable for hole transport (triphenylamine on the surface of A-PDTON nanospheres) and reducing the work function of electrode due to the formation of suitable interfacial dipole (C-PDTON), respectively. We demonstrate the versatility and high compatibility of these two types of the same polymer to organic solar cells, organic light-emitting diodes, and perovskite solar cells, exhibiting comparable or even superior performance compared to the standard device architectures.

CPP 50.12 Thu 12:30 H18

Growth kinetics of gold electrodes used in hybrid solar cells — •Volker Körstgens[1], Adrian Haussmann[1], Franziska C. Löhrer[1], Matthias Schwartzkopf[2], Alexander Hinz[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Hristo Iglev[4], Stephan V. Roth[2], Reinhard Kienberger[4], Franz Faupel[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]DESY, Notkestr. 85, 22607 Hamburg — [3]CAU Kiel, Institut für Materialwissenschaft, Kaiserstr. 2, 24143 Kiel — [4]TU München, Physik-Department, LS Laser- und Röntgenphysik, James-Franck-Str. 1, 85748 Garching

The morphology of the gold electrode established at the metal-polymer interface between gold and the active layer of hybrid solar cells impacts the performance of devices. In this work the active layer consisting of a water-soluble polythiophene and laser-ablated titania nanoparticles including a blocking layer of PEDOT:PSS [1] is investigated. Gold sputter deposition is applied to the layered system and also the respective pure components. To obtain information of gold cluster growth kinetics during the sputter deposition process, in-situ time resolved grazing incidence small angle X-ray scattering (GISAXS) experiments and grazing incidence wide angle X-ray scattering (GIWAXS) are carried out. Different growth regimes of gold clusters are observed from the data analysis for the various films and the influence of surface roughness is discussed. [1] Körstgens et al., Nanoscale 7, 2900 (2015).

CPP 50.13 Thu 12:45 H18

Modelling of photoactive area spreading in unstructured photovoltaic cells — •Mathias Gruber[1,2], Vladislav Jovanov[1], and Veit Wagner[1] — [1]Department of Physics and Earth Sciences, Jacobs University Bremen, 28759 Bremen, Germany — [2]PolyIC GmbH & Co. KG, 90763 Fürth, Germany

Photovoltaic cells incorporating unstructured conductive layers produce a significant amount of additional photocurrent outside the electrode overlap area by photoactive area spreading. This leads to a large error in the extraction of solar cell current density, fill factor and cell efficiency from I-V-measurements. To counteract this effect we present an analytical model which is able to describe the photoactive area spreading effect quantitatively, yielding more accurate results than the conventional shadow masking approach. The presented model only requires layer sheet resistance data and the contact geometry to allow to calculate and remove the spreading current contribution from I-V-measurements of unmasked solar cells. This allows to extract accurate solar cell efficiency and j-V-data, which is demonstrated on the example of unstructured metal mesh based organic solar cells. The presented data demonstrates the problem of the conventional shadow masking approach and shows that our model yields more accurate results down to very low illumination light intensities.

CPP 51: Modeling and Simulation of Soft Matter II (joint session CPP/DY)

Time: Thursday 9:30–12:00 Location: H13

Invited Talk CPP 51.1 Thu 9:30 H13

Systematic Dynamic Coarse-Graining with Memory — Gerhard Jung, Martin Hanke, and •Friederike Schmid — Johannes Gutenberg Universität Mainz, Germany

In soft matter, systematic coarse-graining (CG) approaches often face the problem that the separation of time scales is incomplete, and memory effects become important. One challenge is to extract the CG dynamical equations, namely the memory kernel, from equilibrium all-atom simulations. Another challenge is to devise an algorithm that efficiently deals with pair-memory contributions to the dynamical equations. Such pair-memory interactions may become important, e.g., in dispersions of nanocolloids when the frequency dependence of hydrodynamic interactions cannot be neglected.

The talk will address these two problems. We propose a "generalized Langevin Dynamics" model, which has the form of a generalized Langevin equation with distance-dependent two-particle contributions to the self- and pair-memory kernels. A simulation algorithm is developed that scales linearly with the number of coarse-grained particles. Furthermore, we present a robust iterative method for the accurate reconstruction of memory kernels from dynamic correlation functions.

We apply the method to a suspension of nanocolloids with frequency-dependent hydrodynamic interactions. The GLD simulations perfectly reproduce the dynamics of the underlying fine-grained system and accelerate the simulation by a factor of roughly 10.000.

CPP 51.2 Thu 10:00 H13

Accurate structure-based coarse-graining leads to consistent barrier-crossing dynamics — •Tristan Bereau and Joseph F. Rudzinski — MPI for Polymer Research, Mainz

Structure-based coarse-graining of molecular systems offers a systematic route to reproduce the many-body potential of mean force. Unfortunately, common strategies are inherently limited by the molecular-mechanics force field employed. Here we extend the concept of multi-surface dynamics, initially developed to describe electronic transitions in chemical reactions, to accurately sample the conformational ensemble of a classical system in equilibrium. In analogy to describing different electronic configurations, a surface-hopping scheme couples distinct conformational basins beyond the additivity of the Hamiltonian. The incorporation of more surfaces leads systematically toward improved cross-correlations. The resulting models naturally achieve consistent long-time dynamics for systems governed by barrier-crossing events. [Bereau and Rudzinski, arXiv:1808.05644]

CPP 51.3 Thu 10:15 H13

Mapping multiple timescales in heterogeneous melts with predictive and adaptive subdomains — •Horacio V Guzman[1] and Hideki Kobayashi[2] — [1]Max Planck Institute For Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Theory Research Interest Group, University of Cambridge Lensfield Road Cambridge

Heterogeneous molecular systems can be modeled by means of advanced simulations methods, as it is done with multiscale concurrent representations and non-equilibrium simulations. Interestingly, the heterogeneity of the mentioned systems has a huge potential to map and span time and length scales beyond fully atomistic simulations, since in most cases a subdomain of the simulation box can be tackled with slowly diffusive regime, while other remains in a faster diffusive regime. From this description, a crucial question arises on how to map those heterogeneous time scales without losing the theoretical speedup planned from the method development perspective. Here, we introduce the heterogeneous time-spatial domain decomposition approach which is a combination of an heterogeneity sensitive spatial domain decomposition with a time evolution average of particles' diffusion domainwise estimated. Within this approach, we present the theoretically modeled and results in scaling-laws for the force calculation time, while timewise the subdomains with different diffusivity are adapted by means of the number of neighboring shells to a unique frequency of neighbour list updates. We explore the new approach capabilities, by comparing it with the state-of-the-art spatial domain decomposition techniques.

CPP 51.4 Thu 10:30 H13

Automated detection of many-particle solvation states for accurate characterizations of diffusion kinetics — •Joseph Rudzinski, Marc Radu, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Markov state models are powerful tools for reducing the complexity of molecular dynamics trajectories, but require configuration-space representations that accurately characterize the relevant dynamics. Well-established, low-dimensional order parameters for constructing this representation have led to widespread applications to study conformational dynamics of biomolecules. On the contrary, applications to characterize single-molecule diffusion have been scarce and typically employ system-specific, higher-dimensional order parameters to characterize local solvation states. In this work, we propose an automated method for generating a coarse configuration-space representation, using the coordination numbers about each particle. To overcome the noisy behavior of these low-dimensional observables, we treat the features as indicators of a latent Markov process. The resulting hidden Markov models filter the trajectories of each feature into the most likely latent solvation state at each time step. The filtered trajectories are then used to construct a configuration-space discretization, which accurately describes the diffusion kinetics. The method is validated on a standard model for glassy liquids, where particle jumps between local cages determine the diffusion properties. The resulting models provide quantitatively accurate characterizations of the diffusion constant and also reveal a mechanistic description of diffusive jumps.

CPP 51.5 Thu 10:45 H13

Simulating liquid alkanes from first principles with machine learning potentials — •Max Veit — École Polytechnique Fédérale de Lausanne, 1015 Lausanne, CH — Department of Engineering, University of Cambridge, Cambridge CB2 1PZ, UK

The reliable prediction of the macroscopic properties of molecular liquids requires potential energy surface (PES) models that are not only accurate, but computationally efficient enough to handle large systems and reach long time scales typically inaccessible to explicit quantum-mechanical methods. This work introduces a new approach to the systematic approximation of the first-principles PES of a molecular liquid using the GAP machine learning method [A. Bartók, M. Payne, R. Kondor, and G. Csányi, Phys. Rev. Lett. 104, 136403 (2010)]. By applying machine learning to separately approximate each physical component of the interaction energy in a full many-body framework and with high and controllable accuracy, we can simulate the liquid accurately across a wide range of temperatures and pressures (with the inclusion of quantum nuclear effects) while gaining physical insight into the inner workings of the fluid. Following the recent success of this approach on predicting the equation of state of compressed fluid methane [M. Veit, S. K. Jain, S. Bonakala, I. Rudra, D. Hohl, and G. Csányi, arXiv:1810.10475], I will discuss how this approach can be extended to other molecular liquids with the help of emerging techniques in machine learning potential development, and how these ideas can be applied to other important molecular materials.

CPP 51.6 Thu 11:00 H13

Effective interaction between fillers and their effect on phase separation of polymer blends. — •Alexander Chervanyov — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, DE

Effective interactions between fillers immersed in polymer blends are shown to arise from the interplay between the conventional compressibility mechanism and the mechanism relying on the polymer compositional variations in the vicinity of fillers. By developing and making use of the liquid state theory, we calculate the potentials of the effective interactions acting between fillers having different affinities for polymer species comprising the blend. Further, we study the effect of interacting fillers on phase separation in polymer blends. The calculated shift of the spinodal point and critical temperature are shown to significantly depend on the interactions between fillers and polymers.

Financial support of Deutsche Forschungsgemeinschaft (DFG) through Grant No. CH 845/2-1, is gratefully acknowledged.

15 min. break

CPP 51.7 Thu 11:30 H13

Relative resolution: A multipole approximation at appropriate distances — •Aviel Chaimovich[1], Kurt Kremer[2], and Christine Peter[3] — [1]Max Planck Institute of Colloids and Interfaces, 14476 Potsdam — [2]Max Planck Institute for Polymer Research, 55128 Mainz — [3]University of Konstanz, 78464 Konstanz

Recently, we introduced Relative Resolution as a hybrid formalism for fluid mixtures [1]. The essence of this approach is that molecular resolution switches in terms or relative separation: While near neighbors are characterized by a detailed fine-grained model, far neighbors are characterized by a simplified coarse-grained model. In this presentation, we notably show the comprehensive mathematics of our multiscale algorithm: We cast our Hamiltonian in terms of a multipole approximation at appropriate distances, which allows us for an analytical parameterization between the fine-grained and coarse-grained models. We consequently test the ability of Relative Resolution in describing various nonpolar liquids, in turn, capturing correctly and efficiently the statics and dynamics of many structural correlations and thermal properties across state space. Furthermore, we show that our multiscale approach works best if we switch between the fine-grained and coarse-grained potentials between the primary and secondary coordination shells: At this location, all orientations become negligible in the Hamiltonian. We conclude by discussing how Relative Resolution is the inherent variant, for molecular simulations, of the famous "cell-multipole" approach.

[1] A. Chaimovich, C. Peter, and K. Kremer (JCP, 2015).

CPP 51.8 Thu 11:45 H13

Cononsolvency of thermoresponsive polymers: theory and simulation — •Nico van der Vegt, Swaminath Bharadwaj, Cahit Dalgicdir, and Divya Nayar — Technische Universität Darmstadt, Germany

Cononsolvency of thermoresponsive polymers is an intriguing phenomenon whose molecular-scale mechanism remains elusive ever since it was first reported in the late 1980s. I will present theoretical results and computer simulations which provide a new angle on this question. Significantly, direct cosolvent binding to the polymer is shown to be an entropy-driven process, which leads to polymer dehydration resulting in coil-globule collapse and phase separation in poly(N-isopropyl acrylamide)/water/methanol solutions. Specific cosolvent interactions with the polymer play no role in this mechanism. Instead of that, cosolvent enrichment around hydrophobic groups frustrates hydration of the amide group and induces phase separation. Theoretical arguments and simulation results are furthermore presented which illustrate that direct cosolvent binding is not a necessary requirement for cononsolvency.

D. Nayar, N.F.A. van der Vegt, J. Phys. Chem. B 122, 3587-3595 (2018) N.F.A. van der Vegt, D. Nayar, J. Phys. Chem. B 121, 9986-9998 (2017) C. Dalgicdir, F. Rodriguez-Ropero, N.F.A. van der Vegt, J. Phys. Chem. B 121, 7741-7748 (2017)

CPP 52: Biomaterials and biopolymers I (joint session BP/CPP)

Time: Thursday 9:30–12:45 Location: H10

CPP 52.1 Thu 9:30 H10

A unifying perspective on rigidity in under-constrained materials — •Matthias Merkel[1,3], Karsten Baumgarten[2], Brian Tighe[2], and Lisa Manning[1] — [1]Department of Physics, Syracuse University, Syracuse, NY, USA — [2]Delft University of Technology, Delft, The Netherlands — [3]Centre de Physique Théorique, Université Aix-Marseille, France

We present a novel approach to understand rigidity in under-constrained materials, including sub-isostatic spring networks as well as 2D and 3D vertex models for dense biological tissues. We show that the onset of rigidity is determined by a purely geometric criterion. This allows us to analytically predict the elastic material properties close to the transition, which depend only on few geometric coefficients. We obtain exact expressions for the magnitudes of bulk modulus and shear modulus discontinuities at the rigidity transition, several scaling relations of the shear modulus, and the magnitude of the anomalous Poynting effect. Moreover, we show that the ratio of the excess shear modulus to the shear stress is inversely proportional to the critical shear strain with a prefactor of three, which we expect to be a general hallmark of rigidity in under-constrained materials induced by geometric incompatibility. This could be used in experiments to distinguish whether strain-stiffening as observed for instance in biopolymer networks arises from nonlinear characteristics of the microscopic material components or from effects of geometric incompatibility.

CPP 52.2 Thu 9:45 H10

Heat and light - non-equilibrium tools to break early symmetry — Matthias Morasch[1], Corinna Kufner[2], Stefan Krebs[3], Hannes Mutschler[4], Wolfgang Zinth[5], Dieter Braun[1] und •Christof Mast[1] — [1]Systems Biophysics, LMU Munich, Amalienstr. 54, 80799 Munich, Germany — [2]Harvard-Smithsonian Center for Astrophysics, Harvard University, 60 Garden Street, Cambridge, MA 02138 — [3]Gene Center, LMU Munich, Feodor-Lynen-Straße 25, 81377 Munich, Germany — [4]MPI Biochemistry, Am Klopferspitz 18, 82152 Martinsried, Germany — [5]BMO, LMU Munich, Öttigenstrasse 67, 80538 Munich, Germany

Modern lifeforms perpetuate their highly evolved molecular structures by using them to convert external energy-fluxes for self-replication and evolution. It is an open question how this closed cycle could start around four billion years ago. At that time, no sophisticated enzymes were available to initiate that process from the initially random and racemic pool of early prebio-polymers. We investigate how physical non-equilibria could help this issue by breaking early symmetry and locally enrich oligomer pools with a reduced sequence space and with a homochiral backbone. We are especially interested in the effect of thermal gradients across small water-filled pores and of incident UV-light. Thermal convection chambers could have selected for interacting, hence homochiral, sequences by their thermophoretic and lengthdependent concentration while UV-light is known to damage oligomers in a sequence dependent manner.

CPP 52.3 Thu 10:00 H10

Kinetic Control of Peptide Self Assembly Pathways — •Joshua T. Berryman and Ali Asghar Hakami Zanjani — University of Luxembourg, Luxembourg

Naturally occurring peptides may aggregate to form 3D amyloid-like crystals, or may take on quasi one-dimensional amyloid fibril structures. Mltiple distinct polymorphic structures often exist as subbranches within both the crystallising and fibril-forming pathways, differing either in overall symmetry or in only local conformational degrees of freedom.

We examine and discuss a system of aggregating peptides in which the available polymorphs are observed to differ in the macroscopic chirality of their assembly, with right-twisted fibrils, left-twisted fibrils, and non-twisted crystals forming sometimes even in the same sample. Using atomistic and also coarse-grained calculations we develop a structural and kinetic model for assembly of the amyloid-forming peptides and validate against light scattering and microscopy results [1,2]. We are able to provide a simple analytical expression to predict if a given set of experimental conditions (parameterised by temperature, concentration and pH) will lead to left-handed fibrils, right-handed fibrils or mesoscopic twist-free microcrystals [1].

[1] Reynolds et al., Nat. Comms. 8:1338 (2017)
[2] Lara et al., J. Am. Chem. Soc. 136(12):4732 (2014)

CPP 52.4 Thu 10:15 H10

Early Stage Self Assembly of Flexible Peptides — •Ali Asghar Hakami Zanjani and Joshua T. Berryman — University of Luxembourg, Luxembourg

We use accelerated simulation methods to investigate the early stage nucleation processes of a homologous series of hexapeptides: ILQINS (from hen's egg-white lysozyme), IFQINS (from human lysozyme) and TFQINS (a disease-related mutation in humans). We observe that the majority of initially formed one-dimensional single beta sheets in these systems have antiparallel alignment of peptide strands, in contrast to experimentally observed mature multi-sheet aggregates which have parallel strand alignment in all structures found to date [1-3].

We confirm the stability of the antiparallel aggregates by molecular dynamics simulations showing greater configurational stability for the antiparallel rather than parallel single beta sheets [4]. As mature antiparallel aggregates have not been observed for these systems we assume that such structures represent a kinetic trap, with limited potential to mature into amyloid fibrils or the related microcrystals. The existence of this kinetic trap offers the possibility to control amyloid formation by chemically directing small structures either towards or away from the antiparallel structures, depending if formation of macroscopic aggregates is considered beneficial or harmful.

[1] Reynolds et al., Nat. Comms. 8:1338 (2017)
[2] Lara et al., J. Am. Chem. Soc. 136(12):4732 (2014)
[3] Sievers, PhD Dissertations, (ProQuest, UMI: 3322087, 2008)
[4] Cooper, Beta-Sheet Geometry, (Birkbeck College, 1995)

CPP 52.5 Thu 10:30 H10

The force spectroscopy of a biomimetic polymer in molecular simulations via perturbation theory — •Aviel Chaimovich[1], Christian Leitold[2], Kurt Kremer[3], and Christoph Dellago[4] — [1]Max Planck Institute of Colloids and Interfaces, 14476 Potsdam — [2]University of California, Santa Barbara 93106 — [3]Max Planck Institute for Polymer Research, Mainz 55128 — [4]University of Vienna, 1090 Vienna

It has become a common practice of probing various aspects of biological polymers via force spectroscopy. Considering that many proteins exhibit similar phenomena, we are interested in their corresponding universal signatures. For this purpose, we invoke molecular simulations of a biomimetic polymer: Although this homopolymer is solely based on a bead-spring model with a square-well potential, it is capable of universally capturing the protein-like unfolding of any heteropolymer [1]. Foremost, via the Wang-Landau procedure, we calculate at zero force the free energy as a function of the potential energy of the polymer [2]. We continue via perturbation theory, determining the free energy at nonzero force, applying it on different sets of monomeric sites. We in turn find scaling relations for the activation and transition of the biomimetic unfolding, relating these to various polymeric characteristics (e.g. the radius of gyration). Our findings consequently have important ramifications for protein unfolding.

[1] M. P. Taylor, W. Paul, and K. Binder (PRE, 2009). [2] C. Leitold and C. Dellago (JCP, 2014).

CPP 52.6 Thu 10:45 H10

Heated microbubbles condense and encapsulate prebiotic molecules and enhance ribozymatic activity — •Matthias Morasch[1], Alan Ianeselli[1], Alexandra Kühnlein[1], Saidul Islam[2], Kristian Le Vay[3], Hannes Mutschler[3], Matthew W. Powner[2], Christof B. Mast[1], and Dieter Braun[1] — [1]Systems Biophysics, LMU Munich, Amalienstrasse 54, 80799 München — [2]Department of Chemistry, University College London, 20 Gordon Street, London, WC1H 0AJ, UK — [3]Max-Planck Institute for Biochemistry, Am Klopferspitz 18, 82152, Martinsried, Germany

Interfaces in an otherwise homogeneous system can drastically change local reaction dynamics. Here, we studied microscale water cycles by the application of a temperature gradients to microbubbles in water and found that it triggered a wide range of processes crucial for the origin of life. We could show that biomolecules increase in concentration more than 1000-fold by the capillary flow at the air-water interface.

RNA precursors are found to crystallize around the bubble, allowing for a possible enantiomeric selection, while monomers undergo an enhanced phosphorylation. In the presence of vesicles, nucleic acids are concentrated and encapsulated in vesicle clusters, which are frequently ejected into the bulk solution. In addition, self-complementary RNA is demonstrated to form sequence-pure hydrogels, while the catalysis of the hammerhead ribozyme drastically increased at the interface compared to the bulk. The studied setting is hypothesized to be ubiquitous on early Earth.

15 minutes break.

CPP 52.7 Thu 11:15 H10

Mechanical properties of UV-irradiated collagen fibrils studied with atomic force microscopy — •Marcus Schulze, Melanie Rogge, and Robert Stark — Physics of Surfaces, Materialwissenschaften, TU Darmstadt, Alarich-Weiss-Straße 16, 64287 Darmstadt

Collagen is a widely used component for the synthesis of substrates in the field of Tissue Engineering (TE). Cell adhesion and proliferation on theses substrates is strongly dependent on their mechanical properties which makes a controlled adjustment of these properties a key requirement for a more elaborated substrate design. Among several approaches, the irradiation of the collagen-based substrates with UV light proved itself a valuable technique to modify the mechanics without introducing cytotoxicity. For the evaluation of the influence of UV light on the mechanical properties of collagen fibrils in a liquid environment the atomic force microscope was used. Varying combinations of UV light sources (UV-A, UV-B, and UV-C) and fluids (deionized water and phosphate buffered saline (PBS)) were applied to two kinds of samples. The indentation modulus was measured on surface supported fibrils and a tensile modulus was derived from bending experiments on freely suspended collagen fibrils. Results suggested an increase in modulus within 30 minutes of treatment with UV-B or UV-C light in PBS.

CPP 52.8 Thu 11:30 H10

The effect of surface functionalization and pH on protein-gold nanoparticle interactions — •Brahmaiah Meesaragandla[1,2], Isabel Garcia[3], Luis.M Liz-Marzán[3,4], and Mihaela Delcea[1,2] — [1]Institute of Biochemistry, University of Greifswald, Greifswald, Germany — [2]ZIK HIKE, University of Greifswald, Greifswald, Germany — [3]CIC biomaGUNE and CIBER de Bioingeniería, Biomateriales y Nanomedicina (CIBER-BBN), San Sebastián, Spain — [4]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

In this work, we have investigated the interactions between differently functionalized gold nanoparticles (citrate, PEG-OMe, PEG-COOH, PEG-NH2, and glycan coated AuNPs) and human serum albumin (HSA) with pH using UV-Vis absorption, dynamic light scattering (DLS), and circular dichroism (CD) spectroscopy techniques. HSA exhibit different isomeric forms and undergoes conformational changes at different pH conditions (e.g. pH 3.8, 7.4, and 9.3). Both UV-Vis and DLS measurements have indicated the formation of protein corona. CD spectroscopy studies suggested that HSA conjugated to AuNPs undergoes a change in the secondary structure (decrease in alpha-helix) at various pH for all functionalized AuNPs. This change in protein secondary structure might be due to the type of dominant interaction between NPs and HSA (i.e electrostatic, hydrogen bonding). Our results indicated that both, surface charge and pH of the medium, influences the changes in HSA structure.

CPP 52.9 Thu 11:45 H10

Temperature dependence of the elastic modulus of vapor deposited phospholipid bilayers on solid substrates — Maria J. Retamal[1], •Rodrigo Catalan[2], Marcelo Cisternas[2], Nicolas Moraga[2], Diego Diaz[2], Tomas P. Corrales[3], Mark Busch[4], Patrick Huber[4], Marco Soto-Arriaza[1], and Ulrich G. Volkmann[2] — [1]Faculty of Chemistry and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — [2]Institute of Physics and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — [3]Department of Physics, UTFSM, Valparaiso, Chile — [4]TUHH, Hamburg, Germany

Phospholipid membranes (PMs) play a key role in most physiological processes. Besides the function of membrane proteins, changes in the fluidity of the phospholipid membrane are crucial in the permeability of certain molecules, such as oxygen or glucose. We analyze with Atomic Force Microscopy (AFM) and Surface Force Spectroscopy (SFS) the temperature dependence of Young's modulus (YM) of non-functional PMs (DPPC, DMPC and DSPC). Phospholipids were vapor-deposited in high vacuum onto silicon substrates. AFM measurements in liquid confirm the self-assembly of the phospholipid bilayer and YM measurements with SFS indicate the main transitions of the phospholipid bilayers. We show that PMs made by PVD in high vacuum preserve their structure and mechanical properties after proper hydration. This study opens new pathways to assemble phospholipid mixtures by means of solvent-free membrane formation. Acknowledgements: FONDECYT Nos. 3160803 (MJR), 1180939 (UGV), 1171047 (MSA) and 11160664 (TPC), CONICYT Fellowship (MC) and CONICYT-PIA ACT 1409.

CPP 52.10 Thu 12:00 H10

Sequence effects on size, shape, and structural heterogeneity in Intrinsically Disordered Proteins — •Upayan Baul[1], Debayan Chakraborty[2], Mauro L. Mugnai[2], John E. Straub[3], Devarajan Thirumalai[2], and Joachim Dzubiella[1] — [1]Institute of Physics, Albert-Ludwigs-University of Freiburg, Hermann-Herder-Strasse 3, 79104 Freiburg, Germany — [2]Department of Chemistry, The University of Texas at Austin, Austin, Texas 78712 — [3]Department of Chemistry, Boston University, Boston, Massachusetts 02215

Intrinsically disordered proteins (IDPs) lack well-defined three-dimensional structures, thus challenging the archetypal notion of structure-function relationships in proteins. We present the development of a coarse grained simulation model that quantitatively characterizes the structural features of IDPs as a function of sequence and length (N_T). For diverse IDP sequences, with N_T ranging from 24 to 441, our simulations not only reproduce the radii of gyration (R_g) obtained from experiments, but also predict the scattering intensity profiles in near quantitative agreement with Small Angle X-ray Scattering experiments. While R_g values are well-described by the standard Flory scaling law, $R_g = R_0 N_T^{\nu}$, with $\nu = 0.588$, analyses reveal that the extent of conformational heterogeneity for IDPs is highly sequence-dependent, even though ensemble-averaged properties suggest synthetic polymer-like behavior in a good solvent. In conclusion, we comment on the effects of external stimuli such as salt concentration and temperature on the conformational properties of polypeptide sequences.

CPP 52.11 Thu 12:15 H10

Co-survival and competition relationship between bacteria analyzed in millifluidic droplet sequence — •Xinne Zhao[1], Larysa Baraban[1,2], and Gianaurelio Cuniberti[1,2] — [1]Institute of Materials Science and Max Bergmann Center of Biomaterials Dresden, TU Dresden, Dresden, Germany — [2]Center for advancing electronics Dresden, cfaed, Dresden

Analysis of living systems, e.g. bacterial or cells populations plays significant role in fundamental research of population diversity, and evolution.1 Here, we present an optical detection system, combining the encapsulation of bacteria into numerous emulsion droplets to monitor their long term behavior and their relationship in co-culture environment. The bacteria we choose here are BFP E.coli and YFP E.coli which can express blue fluorescence and yellow fluorescence separately under different light illuminations. By detecting the emission wavelength from different E.coli, we can obtain the information of growth state of each bacteria strain. Compared to the classical cell culture methods, the strategy we use here can avoid the influence of getting sample during bacteria growing, as well achieve real-time and automatic monitoring. In order to find out the co-survival and mutual competition relationship between the two bacteria strains, we plan to get the reference growth curve of individually culturing both strains, co-culture them with different initial cell concentration ratios, add antibiotics, as well as compare their maximum cell concentration and generation time.

[1] R. Illing et al, Biomicrofluidics, 2016, 10, 024115.

CPP 52.12 Thu 12:30 H10

Collagen gels determine the viscoelastic properties of tissue without hindering the diffusion of the aqueous solvent — Frank Sauer[1], Linda Oswald[1], Angela Ariza de Schellenberger[3], Heiko Tzschätzsch[3], •Felix Schrank[3], Tony Fischer[2], Jürgen Braun[4], Claudia T. Mierke[2], Rustem Valiullin[5], Ingolf Sack[3], and Josef A. Käs[1] — [1]Soft Matter Physics Division,Peter Debye Institute for Soft Matter Physics, Leipzig, Germany — [2]Biological Physics Division,Peter Debye Institute for Soft Matter Physics, Leipzig, Germany — [3]Department of Radiology, Charité-Universitätsmedizin, Berlin, Germany — [4]Institute of Medical Informatics,Charité-Universitätsmedizin, Berlin, Germany —

[5]Applied Magnetic Resonance, Felix Bloch Institute for Solid State Physics, Leipzig, Germany

Collagen accounts for the major extracellular matrix component in many tissues providing mechanical support for cells. Little is known whether water diffusion interacts with viscoelastic properties of tissues. We are combining highfield MR based diffusion measurements, novel compact tabletop MRE and confocal microscopy in collagen networks of different cross-linking states (untreated versus additional treatment with glutaraldehyde). The MRE-measured shear modulus is sensitive to interactions on the intrafiber level (e.g. fiber stiffness) and is able to depict the pronounced transition from viscous-soft to elastic-rigid gel properties. 3D pore size analysis indicate an unaltered overall network structure and MR based diffusion measurements further allude that there is free extracellular diffusive water transport in connective tissue.

CPP 53: Perovskite and Hybrid Photovolatics I (joint session HL/CPP)

Time: Thursday 9:30–13:00 Location: H36

CPP 53.1 Thu 9:30 H36

Effects of Masking on Open-Circuit Voltage and Fill Factor in Solar Cells — •Kristofer Tvingstedt[1], David Kiermasch[1], Lidón Gil-Escrig[2], and Henk J. Bolink[2] — [1]Experimentelle Physik VI Julius Maximilians Universität Wûrzburg — [2]Instituto de Ciencia Molecular, Universidad de Valencia, C/Catedrático J. Beltrán 2, 46980 Paterna, Spain

Guidelines for the correct measurement protocol of novel photovoltaic technologies such as perovskites are now becoming more frequent in literature. This because, as will be confirmed in this talk, it is not straightforward to correctly measure the true efficiency parameters of these and many other novel solar cells. This is particularly the case for small area research devices which are prone to overestimate the short circuit current density, due to edge effects of various types. To reduce the inaccuracy of current density determination, the common recommended practice is to utilize masks with well-defined apertures, often smaller than the device active area. Herein we show both experimentally and theoretically that this common practice, however, leads to erroneous determination of both open-circuit voltage and fill factor, which are figures of merit of equal importance to the short-circuit current density. Although the errors induced in voltage and fill factor by using a mask are generally smaller than what the errors in current can amount to when not using a mask, they are on the other hand omnipresent and can be quite well described.

CPP 53.2 Thu 9:45 H36

Enhanced stability and optical properties of perovskite nanocrystals encapsulated in block copolymer micelles — •Hyowon Jeong, Carola Lampe, Moritz Gramlich, and Alexander S. Urban — Nanospectroscopy Group, Department of Physics, Ludwig-Maximilians-Universität München (LMU), Amalienstraße 54, 80799, Munich, Germany

Recently, lead halide perovskites in the form of colloidal nanocrystals (NCs) have emerged as promising candidates for use in light-emitting and photovoltaic devices. High photoluminescence quantum yields as well as size- and consequently band gap- tuning are enabled by a facile synthesis and the natural defect tolerance of the material. However, to exploit these fascinating properties, long-term stability of the NCs under different conditions is necessary. Here, a novel synthesis is introduced, where methylammonium lead iodide (MAPbI3) NCs are grown inside of micelles formed by block copolymers, which protect the NCs from the environment and greatly enhance their lifetime. In addition, the optoelectronic properties of the encapsulated NCs will be discussed based on single NC spectroscopy results.

CPP 53.3 Thu 10:00 H36

Energy transfer in films of thickness-tunable CsPbBr3 nanoplatelets — •Andreas Singldinger, Moritz Gramlich, Carola Lampe, and Alexander S. Urban — Nanospectroscopy Group, Department of Physics, Ludwig-Maximilians-Universität München (LMU), Amalienstrasse 54, 80799 Munich, Germany

In recent years, lead halide perovskites have rapidly attracted attention not only in their bulk but also in their nanocrystal form. Various synthetic routes yield highly luminescent nanocrystals of different shapes and sizes and consequently enable band gap tuning through quantum confinement effects. A novel synthesis now allows the growth of quantum-confined CsPbBr3 nanoplatelets (NPLs) with an adjustable thickness ranging from two to six unit cells. These NPLs show strong blue emission induced by a fast radiative decay of excitons. For efficient electroluminescence, however, insight into energy and charge transfer between these NPLs is crucial. Here, we look at two energy transfer processes in perovskite nanocrystal films. Firstly we study energy transfer between NPLs of different bandgaps, via time-resolved photoluminescence-spectroscopy. Secondly we investigate diffusion of photo-excited excitons in films comprising NPLs of a single thickness.

CPP 53.4 Thu 10:15 H36

Ultrafast phonon dynamics in lead halide perovskite — •Hong-Guang Duan[1,2,3], Vandana Tiwari[1], 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

Hybrid organic-inorganic perovskites has gathered much attention owing to their unprecedented success in photovoltaics. To unravel the secrets to this success, we have studied the ultrafast dynamics of lead halide perovskites using heterodyne-detected transient grating and two-dimensional spectroscopy in thin films at room temperature. We distinctly observe the ground and excited state vibrational modes corresponding to organic and inorganic sub-lattices. The interplay of strongly coupled dominant vibrational modes to ultrafast carrier generation process will be discussed. Our experiments also unravel the role of organic cations in the ultrafast dynamics after photoexcitation.

CPP 53.5 Thu 10:30 H36

Effect of the organic cation in halide perovskites on vibrations in the far-infrared region: a combined theoretical-experimental study — •Christian Gehrmann[1], Michael Sendner[2,3], Sebastian Beck[2,3,4], Robert Lovrincic[2,4], and David A. Egger[1] — [1]Institute of Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]InnovationLab, 69115 Heidelberg, Germany — [3]Kirchhoff Institute for Physics, Heidelberg University, 69120 Heidelberg, Germany — [4]Institute for High Frequency Technology, TU Braunschweig, 38106 Braunschweig, Germany

Halide perovskites (HaPs) are intriguing optoelectronic materials. In particular, hybrid organic-inorganic HaPs have attracted much interest as possible solar-cell materials. Since phonons might be the dominant source of scattering for charge carriers at room temperature, special efforts should be made to understand lattice dynamics in HaPs. While the internal vibrations of the organic cation are mainly in the mid-infrared region, we study the impact of the cation on vibrations in the far-infrared region by comparing the hybrid MAPbBr3 to the all-inorganic CsPbBr3. To this end, we present lattice dynamics calculations, based on density functional theory. The theoretical results are compared to experimental data obtained from far-infrared spectroscopy. Using reflectance measurements, we can even present experimental results related to the LO phonons which are not infrared active, but inherently contained in our calculations.

CPP 53.6 Thu 10:45 H36

Density-functional-theory modeling of point defects in halide-perovskite alloys — •Li Jingrui and Patrick Rinke — Department of Applied Physics, Aalto University, Finland

Perovskite solar cells (PSCs) are a promising emergent technology, because their photo-conversion-efficiency has been increasing rapidly in recent years. In these cells, the photoabsorbing material is a hybrid (organic-inorganic) halide perovskites (ABX$_3$), that is usually grown with low-temperature solution-based synthesis. This synthesis method introduces many point defects, that may critically affect the electronic and structural properties of the PSCs. To gain microscopic insight, we used density-functional-theory to study a series of point defects of halide-perovskite alloys with ion-mixing at A (methylammonium, Cs and Rb), B (Pb and Sn) and X (I, Br and Cl) sites. The considered defects include A- and X-site vacancies and native interstitials in different charge states, as well as K and H impurities. For each model system, a $4 \times 4 \times 4$ perovskite supercell was relaxed using the PBEsol exchange-correlation functional. Then the electronic structure and defect formation energy were calculated using the hybrid HSE06 functional. Our results indicate that the defect formation energy sensitively depends on the phase and composition of halide perovskites. For halogen vacancies, the $+1$ state that has very small impact on the electronic structure is the most stable in a large Fermi-energy range. Only within the strongly n-type doped region, neutral or negatively-charged halogen vacancies will be formed, which introduce states in the band gap and significantly limit the PSC efficiency.

15 min. break

CPP 53.7 Thu 11:15 H36

Calculating structural properties of halide perovskites: Influence of the computational approach — •Hubert Beck, Christian Gehrmann, and David A. Egger — Institute of Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Hybrid organic-inorganic halide perovskites (HaPs) have shown promising results in the development of new optoelectronic devices. Density functional theory (DFT) based first-principles calculations can address several of the open questions for these systems. For many of those calculations it is of vital importance to understand, which of the various microscopic effects in different DFT-related approximations play an important role. Here, we present an investigation of the importance of various theoretical aspects in the DFT calculations of the structural properties for the prototypical case of $MAPbI_3$. The main focus is on a comparison of calculations varying the DFT functional, the account of dispersion forces as well as the inclusion of spin-orbit coupling. The relative effect for the calculations of structural properties of $MAPbI_3$ is evaluated by comparing our computed unit-cell volumes and bulk moduli to results of experiments. Finally, we also present results on the impact of temperature-induced structural fluctuations on calculating the structural properties of $MAPbI_3$.

CPP 53.8 Thu 11:30 H36

Identification of trap states by photo-induced transient spectroscopy in metal halide perovskites — •Mathias Fischer[1], Andreas Baumann[2], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Defects in perovskite solar cells ar often related to a reduced device performance. A common method for the characterization of defects in conventional semiconductors is the deep level transient spectroscopy (DLTS). This technique is based on a modulation of the depletion layer width by injecting charge carriers, mostly by applying voltage pulses. Due to electrical field screening in the device, redistribution of mobile ions and relatively low conductivity of organic transport layers, particularly when studying the device at low temperatures, charge carrier injection via voltage pulses is often difficult. This limitation can be mostly overcome by charge carrier injection charges via optical pulses, which enables us to record a rich trap spectrum over the broad temperature range down to 30 K. We apply this technique, which is also known as photo induced-transient spectroscopy (PITS), to perovskites of various compositions and compare the results with complementary techniques, such as thermal admittance spectroscopy and TSC. We show that multiple additional trap states can be observed when optical pulses instead of voltage pulses are used for injection of charges into the device.

CPP 53.9 Thu 11:45 H36

Identifying recombination dynamics in efficient perovskite solar cells with transient optoelectrical techniques via active layer thickness alteration — •David Kiermasch[1], Lidón Gil-Escrig[2,3], Andreas Baumann[4], Henk J. Bolink[2], Kristofer Tvingstedt[1], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Instituto de Ciencia Molecular, Universidad de Valencia, 46980, Paterna, Spain — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, 12489 Berlin — [4]Bavarian Center for Applied Energy Research (ZAE Bayern) Bayern, 97074 Würzburg

Quantifying charge carrier recombination processes leading to energy losses in perovskite solar cells is of crucial importance for further improvements. Usually time-resolved photoluminescence (PL) is used to study charge carrier recombination, since electrical techniques are often limited by large capacitance values due to thin film layers and mostly short charge carrier lifetimes. By optimizing both the active layer thickness and the surrounding transport layers, we identified bulk dynamics using the combination of Transient Photovoltage (TPV) and Charge Extraction (CE) in $MAPbI_3$ solar cells with V_{oc}'s above 1.1 V and efficiencies up to 18 %. This allows us to assign loss processes to be mainly of Shockley-Read-Hall and free-carrier recombination type in line with PL studies on pure films. Our work also shows that increasing the perovskite thickness, advantageous to achieve high photocurrents, does not affect the recombination dynamics significantly confirming the high quality of the vacuum processed solar cells studied herein.

CPP 53.10 Thu 12:00 H36

Describing the Optoelectronic Properties of Halide Perovskites with a Tight Binding Approach — •Maximilian J. Schilcher[1], Matthew Z. Mayers[2], Liang Z. Tan[3], David R. Reichman[2], and David A. Egger[1] — [1]Institute of Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Chemistry, Columbia University, New York, NY 10027, USA — [3]Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

The intriguing optoelectronic properties of halide perovskites (HaPs) have invoked the development of new solar cells with enormous power conversion efficiencies. However, it is still not understood how these optoelectronic properties can emerge despite the remarkably soft lattice of HaPs. Theoretical calculations reveal important structure-function relations, yet are often limited by computational costs. We aim for developing theoretical tools that enable the simulation of HaPs with low computational costs, since for the calculation of realistic properties large super cells are often required. Their simulation via more conventional theoretical tools, such as density functional theory (DFT), can be challenging or even impossible. An efficient approach to model large-scale system sizes is the tight binding (TB) formalism. Here, we develop a TB parametrization for the HaP methylammonium lead bromide by projecting the Bloch wave functions on the basis functions corresponding to specific orbital sites of the atoms. This allows us to examine the impact of ionic composition and the effect of dynamical structural distortions on the optoelectronic properties of HaPs.

CPP 53.11 Thu 12:15 H36

A completely solvent free route for hybrid perovskite film processing based on pressure treatment of perovskite powders - decoupling material synthesis and film formation — Nico Leupold[2], Maximilian Schulz[1], Konstantin Schötz[1], Ralf Moos[2], and •Fabian Panzer[1] — [1]Soft Matter Optoelectronics — [2]Department of Functional Materials, all University of Bayreuth, Bayreuth, 95440, Germany

Even though hybrid perovskites have undergone a remarkable development within the last years, state of the art processing approaches such as solution processing or evaporation suffer from an intrinsically high complexity, as the perovskite crystallization and its film processing happen simultaneously and are inextricably interconnected. Here we present an alternative, entirely dry processing approach, decoupling perovskite crystallization and film formation, by using readily prepared perovskite powders and produce films by appropriate mechanical pressure treatment. We show how a mechanochemical synthesis by ball milling allows to produce a wide range of phase pure and highly stable perovskite powders with a high flexibility in processing and we address the impact of milling parameters on the powder properties. Using these powders, we demonstrate how the used pressure and the powder microstructure, i.e. particle size and stoichiometry affect the mechanical stability, compactness and surface roughness of the pressed layers. We further address how specific temperature treatment during the pressing step can improve the properties of the pressed layer, and show their capability to be used in perovskite based optoelectronic devices.

CPP 53.12 Thu 12:30 H36

Ultrafast two-dimensional electronic spectroscopy of CsPbBr3 perovskite crystals — •Xuan Trung Nguyen[1], Daniel Timmer[1], Yevgeny Rakita[2], David Cahen[2], Antonietta De Sio[1] und Chirstoph Lienau[1] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — [2]Weizmann Institute of Science, Israel

Halide perovskites are attractive as cost-effective materials for developing highly efficient solar cells. Many research discussed about generation of excitons and free charges in halide perovskites under optical excitation. However, the role of excitons and their interplay with free charges for the optoelectronic and transport properties is not yet clear. Here we use two-dimensional electronic spectroscopy (2DES), with 10-fs-time resolution, to study the initial dynamics of optical excitations in single crystals of CsPbBr3. Upon excitation, we observe bleaching of the exciton resonance as diagonal peak and a cross-peak suggesting their interaction with free charges. Interestingly, the exciton peak vanishes within only ˜20 fs and an intense elongated cross-peak persists for several ps. These results suggest efficient screening of exciton by free charges and highlight the importance of many-body interactions in the ultrafast dynamics of halide perovskites crystals.

CPP 53.13 Thu 12:45 H36

Exploring the stability of halide perovskite alloys by combining density-functional theory and machine learning — •Guo-Xu Zhang[1,2], Lauri Himanen[1], Jingrui Li[1], and Patrick Rinke[1] — [1]Department of Applied Physics, Aalto University, Finland — [2]School of Chemistry and Chemical Engineering, Harbin Institute of Technology, China

Halide perovskites (ABX_3) have attracted considerable attention in recent years due to their breakthrough performance as photovoltaic materials in perovskite solar cells (PSCs). We here consider the materials space of perovskites spanned by A = Cs and Rb, B = Sn and Pb, and X = Cl, Br, and I. Since this space is too large to peruse with density-functional theory (DFT) alone, we combine DFT with machine learning. We use the recently proposed many-body tensor representation (MBTR) [1] as structural descriptor. We then train a kernel ridge regression (KRR) model for fast energy prediction with DFT energies for 2×2×2 and 4×4×4 perovskite supercell models of varying composition. We analyse the effect of MBTR parameters on the KRR learning quality and then use KRR to explore the vast alloy space. We compute the convex-hull of several binary alloy series, for example $Cs_xRb_{1-x}PbI_3$, $CsPb_xSn_{1-x}I_3$, and $Cs_xRb_{1-x}Pb_ySn_{1-y}Cl_{z_1}Br_{z_2}I_{3-z_1-z_2}$. Our prediction accuracy for the cohesive energy of different alloys is as low as few meV/atom. This suggests that KRR in combination with the MBTR can be used to speed up the discovery of stable halide perovskite alloys.

[1] Huo and Rupp, arXiv 1704.06439.

CPP 54: Active Matter II (joint session DY/CPP)

Time: Thursday 10:00–12:45 Location: H19

CPP 54.1 Thu 10:00 H19

Self-propelled Janus particles in evaporating droplets — Maziyar Jalaal[1,2], Borge Ten Hagen[1], Hai Le The[3], Christian Diddens[1], Detlef Lohse[1,2], and •Alvaro Marin[1] — [1]Physics of Fluids, University of Twente, The Netherlands — [2]Max-Planck Center for Complex Fluid Dynamics, University of Twente, The Netherlands — [3]BIOS-Lab on a Chip, University of Twente, The Netherlands

According the kids britannica encyclopedia: “Living things have the ability to move in some way without outside help.”. Following this precise definition, artificial self-propelled particles are not alive, but they almost are since they move taking advantage of chemical/physical reactions or more complex interactions with their environment. Such active particles have been developed and thoroughly characterized in recent years *in vitro*: in either quiescent liquid media or stationary flow fields. However, in most situations *living things* encounter unsteady flows and interfaces of different types. To approach more realistic situations, we choose to study the dynamics of self-propelling Janus particles in evaporating droplets. Our system consists on polysterene-platinum Janus colloids immersed in a sessile droplet containing an hydrogen peroxide solution. The system is analyzed using three-dimensional particle tracking measurements and numerical simulations of the nontrivial fluid flow within the evaporating droplet. To our surprise, the dynamics of the active particles turns to be extremely rich due to several mechanisms as the proximity to interfaces, concentration gradients and evaporation-driven flows.

CPP 54.2 Thu 10:15 H19

Tuning propulsion modes in active emulsions — •Corinna C. Maass, Babak Vajdi Hokmabad, and Kyle A. Baldwin — Max-Planck-Institut für Dynamik und Selbstorganisation

Single cell organisms show a variety of swimming behaviours: e.g. persistent, helical, run-and-tumble or switch-and-flick, all dependent on intricate biophysical machinery and serving various strategies of navigation, e.g. persistence against external flow, efficiency of gradient sensing or expanding their range of exploration. Their locomotion has to adapt to low Reynolds numbers, highly viscous or non-Newtonian environments. An important aspect to the construction of biomimetic model swimmers is to mimic as many of those strategies as possible, based on simple principles of non equilibrium physics without requiring intricate biochemical machinery. Here, we investigate the dynamics of active droplets dependent on the viscosity of the bulk phase. We can tune their propulsion from almost ballistic persistence over a quite diffusive “run-and-spiral” mode to a “stop-and-go” behaviour that is noisy on short, but persistent on long time scales, simply by changing the composition of the bulk phase with a varying fraction of glycerol. Such unsteady swimming is caused by a dynamic instability in the chemical and hydrodynamic fields around the droplets which we have mapped simultaneously via multichannel fluorescent video microscopy.

CPP 54.3 Thu 10:30 H19

Swimming droplet in confined geometries — •Charlotte de Blois, Mathilde Reyssat, and Olivier Dauchot — Gulliver Laboratory, UMR CNRS 7083, ESPCI Paris, PSL University

Micro-swimmers rarely evolve in a 3D infinite and unbounded medium. Instead, they are confined by external geometries which strongly modify their behavior. There is however no exact theoretical knowledge of the flow fields in this context and experimental data are scarce. Here we consider a swimming water droplet [1], denser than the continuous phase, in confined geometries from 2D motion parallel to a bottom wall to 1D motion in capillaries. [1] Izri et al. PRL 113, 248302 (2014).

CPP 54.4 Thu 10:45 H19

Active liquid crystal shells: stability and dynamics — •Babak Vajdi Hokmabad, Kyle A. Baldwin, Carsten Krüger, Christian Bahr, and Corinna C. Maass — Max Planck Institute for Dynamics and Self-organization

Production of controllable, active microcapsules is of great interest in synthetic biology and microchemistry. Inactive microcapsules, also known as double emulsions or droplet shells, are already widely used as artificial cells, micro-reactors, and in food and drug applications. However, combining activity, stability, and control remains a significant challenge. Using established concepts of active emulsions we have developed a new approach to the problem of encapsulation by using nematic active double emulsions, where a solubilization mechanism induces activity and the molecular nematicity provides stability. We show that using a nematic liquid crystal as the shell material and imposing homeotropic anchoring at both interfaces will result in a nematoelastic force on the internal droplet and act as a topological barrier against the coalescence of the core droplet with the outer phase. We further present a peculiar self-propulsion mode where the interplay of spontaneous symmetry breaking and autochemotaxis results in a ”shark-fin meandering” motion of the shell in a 2D-confined geometry and a helical swimming in 3D. This behavior can be controlled or switched off by introducing chemical gradients, topographical guidance or through shell topology variation.

CPP 54.5 Thu 11:00 H19

Flow of active granular particles through a bottleneck — •Tina Hanselka and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg

We use screws performing a self-propelled motion on a vibrated plate as a simple model to analyze the collective behavior of active matter systems passing through a constriction. For this we employ a slight tilt of the plate to simulate an effective gravity and to give the particles a preferred direction towards the bottleneck, and we examine the characteristics of flow and clogging as a function of geometrical and driving parameters.

15 min. break

CPP 54.6 Thu 11:30 H19

Autonomous engines driven by active matter: Energetics and design principles — •Patrick Pietzonka[1], Etienne Fodor[1], Christoph Lohrmann[2], Michael E. Cates[1], and Udo Seifert[2] — [1]Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK — [2]II. Institut für Theoretische Physik, Universität Stuttgart, Germany

We explore how active matter in a non-equilibrium steady state can autonomously deliver mechanical work against a constant mechanical force or torque. For this purpose, we consider systems that contain one or several active components and a single passive component that is asymmetric in its geometrical shape or its interactions. Generally, one expects that such an asymmetry leads to a persistent, directed current in the passive component, which can be used for the extraction of work. We show which two-dimensional shapes of the passive particle are best suited for the extraction of work. Approximating their effect on the dynamics of the particles leads to analytical results for the power and efficiency. A mean field approach reveals that the interaction with the passive particle can mediate cooperativity between otherwise non-interacting active particles, leading to an enhanced efficiency.

CPP 54.7 Thu 11:45 H19

Pair-distribution function of active Brownian particles in three spatial dimensions* — •Stephan Bröker, Jens Bickmann, and Raphael Wittkowski — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

The pair-distribution function is a key quantity for analyzing many-particle systems. It characterizes the particle configuration and is often required when describing such systems via field theories. While for passive particles this correlation function has been extensively studied and analytical approaches exist for it, little is known about the pair-distribution function for active particles.

Therefore, based on Brownian dynamics simulations, we have determined the full pair-distribution function of a homogeneous system of spherical active Brownian particles in three spatial dimensions. The full pair-distribution function takes not only the positions, but also the orientations of the particles into account and depends additionally on the speed and mean concentration of the particles. We discuss the structure of this function and present an analytical expression that represents the function with good accuracy. In addition, we present a new field theory for active Brownian particles that uses this expression. Our results will be beneficial for future research that aims at describing the collective dynamics of active Brownian particles or at developing methods for predicting the pair-distribution function in nonequilibrium many-particle systems.

**Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1*

CPP 54.8 Thu 12:00 H19

Locomotion of self-acoustophoretic colloidal particles — •Johannes Voss and Raphael Wittkowski — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

During the last two decades, a large number of different realizations of artificial self-propelled colloidal particles has been developed. A particularly advantageous realization is given by self-acoustophoretic colloidal particles, which exhibit self-propulsion when they are exposed to ultrasound. Compared to other types of artificial self-propelled particles, they have a biocompatible propulsion mechanism and can move in various liquids and soft materials. Furthermore, they can permanently be supplied with energy and, via the ultrasound intensity, it is even possible to adjust their speed. This makes self-acoustophoretic particles relevant for potential applications in, for example, medicine and materials science. Up to now, however, these particles have not been investigated in depth. Even the details of their propulsion mechanism are still unclear.

Therefore, based on direct computational fluid dynamics simulations, we have extensively studied the locomotion of self-acoustophoretic colloidal particles. We present results that explain the self-propulsion mechanism of these particles and how their locomotion depends on the shape and other properties of the particles. Our results are helpful especially for future experimental work further investigating or applying self-acoustophoretic colloidal particles.

CPP 54.9 Thu 12:15 H19

Pairing, waltzing and scattering of chemotactic active colloids — •Suropriya Saha[1], Sriram Ramaswamy[2], Ramin Golestanian[1], and Ramin Golestanian[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17 37077 Göttingen — [2]Indian Institute of Science, Bangalore, India

Two chemotactic active colloids, which can rotate their polar axis to align with an imposed chemical gradient, form bound states by cancellation of velocities. Their interactions are dynamical in origin, with contributions from self-propulsion and phoretic response to chemical field generated by each other, are thus non-central and non-reciprocal. Two swimmers remain bound at long times when the chemotactic response of at least one of the swimmers is positive, i.e. it rotates its polar axis to point up a linear gradient. These bound states fall in two broad categories *(i) active dimers, separation fixed and polar axes orient along a line (ii) periodic orbits, relative inclination of the polar axes fixed, while the centre of mass executes cyclic motion. Chemotactic swimmers unbind and scatter away depending on initial conditions or with an increase of self-propulsion; while mutually anti-chemotactic swimmers always scatter away. These findings are summarized in state diagrams and representative trajectories are calculated to illustrate the rich dynamics. For the special case of a swimmer moving in a localised source of fuel, the fixed points underlying the bound states and the bifurcations that lead to transition between from one type of final state to another are classified.

CPP 54.10 Thu 12:30 H19

Diffusion of active particles in a complex environment: role of surface scattering — •Theresa Jakuszeit, Ottavio A. Croze, and Samuel Bell — Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, U.K

Microfluidic experiments have shown that self-propelled particles can slide along the surface of a circular obstacle without becoming trapped over long times for obstacles below a critical radius. Using simulations and theory, we study the impact of different boundary conditions on the diffusive transport of active particles in a lattice of such obstacles. We find that particle dynamics with sliding boundary conditions can result in large diffusivities even at high obstacle density, unlike classical specular reflection as in the Lorentz gas. These dynamics are very well described by a model based on Run-and-Tumble particles with microscopically derived tumbling frequencies and reorientation functions arising from obstacle-induced tumbles. This model, however, fails to describe fine structure in the diffusivity at high obstacle density predicted by simulations. Using a simple deterministic model, we show that this structure results from particles being guided by the lattice.

CPP 55: Physics of Self-Organization in DNA Nanostructures (joint session CPP/BP)

Time: Thursday 12:15–13:00 Location: H13

CPP 55.1 Thu 12:15 H13

Synthetic cells: Bottom-up assembly with DNA nanotechnology — •Kerstin Göpfrich[1,2], Kevin Jahnke[1,2], Ilia Platzman[1,2], and Joachim P. Spatz[1,2] — [1]Max Planck Institute for Medical Research, Department of Cellular Biophysics, Jahnstraße 29, D 69120, Heidelberg — [2]Department of Biophysical Chemistry, University of Heidelberg, Im Neuenheimer Feld 253, D 69120 Heidelberg

Bottom-up synthetic biology has been successful at isolating components from cells and reconstituting subcellular functions inside compartments. Progress towards a fully functional synthetic cell, however, requires strategies to recombine and arrange a multitude of components in space and time. We therefore propose to merge two precision technologies, namely microfluidics and DNA nanotechnology, to position and manipulate components in synthetic cells. In particular, we demonstrate that DNA can be used as a near-universal tool for responsive and programmable compartment functionalization. Our method relies on the self-assembly of single-stranded cholesterol-tagged DNA handles, which provide an addressable anchoring point for complementary DNA carrying an arbitrary functional group. Using this DNA handle approach, we demonstrate the stimuli-responsive attachment of reactive groups, DNA nanostructures, microspheres, an actin cortex and even living cells to the periphery of surfactant-stabilized droplets. We further employ DNA to construct functional components, including a pH-responsive DNA-based cytoskeleton mimic, which serves as a stabilizing cortex inside synthetic cells.

CPP 55.2 Thu 12:30 H13

DNA-Assembled Plasmonic Waveguides for Nanoscale Light Propagation — •Thorsten-Lars Schmidt — Department of Physics, Kent State University, Kent, OH, USA — cfaed, TU Dresden, Germany

Plasmonic waveguides consisting of metal nanoparticle chains can localize and guide light well below the diffraction limit, but high propagation losses due to lithography-limited large interparticle spacing have impeded practical applications. We previously demonstrated a robust DNA-origami-based self-assembly pipeline of monocrystalline gold nanoparticles. More recently, we demonstrated that this method allows the interparticle spacing to be decreased below 2 nm, thus reducing propagation losses to 0.8 dB per 50 nm at a deep subwavelength confinement of 62 nm ($\tilde{}\lambda/10$). We characterize the individual waveguides with nanometer-scale resolution by electron energy-loss spectroscopy. Light propagation towards a fluorescent nanodiamond is directly visualized by cathodoluminescence imaging spectroscopy on a single-device level, therefore realizing nanoscale light manipulation and energy conversion. Simulations suggest that longitudinal plasmon modes arising from the narrow gaps are responsible for the efficient waveguiding. With this scalable DNA origami approach, micrometer-long propagation lengths could be achieved, enabling applications in information technology, sensing and quantum optics.

CPP 55.3 Thu 12:45 H13

Functionalized DNA Origami Nanostructures for Molecular Electronics — •Turkan Bayrak[1], Jingjing Ye[2], Richard Weichelt[3], Amanda Reyes[4], Alexander Eychmüller[3], Enrique Samano[4], Ralf Seidel[2], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany. — [2]Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Germany. — [3]Physikalische Chemie, Technische Universität Dresden, Germany. — [4]Centro de Nanociencias y Nanotecnología, Ensenada, México.

The DNA origami method provides a programmable bottom-up approach for creating nanostructures of any desired shape, which can be used as scaffolds for nanoelectronics and nanophotonics device fabrications. Based on this technique, the precise positioning of metallic and semiconducting nanoparticles along DNA nanostructures can be achieved. In this study, various DNA origami nanostructures (nanomolds, nanotubes and nanosheets) are used for the fabrication of nanoelectronic devices. To this end, gold nanoparticles, semiconductor quantum dots/rods are used in/on the DNA origami structures to create nanowires and transistor-like devices. The DNA origami nanowires and transistors were electrically characterized from room temperature (RT) down to 4.2K. Temperature-dependent characterizations of wires were performed in order to understand the dominant conduction mechanisms. Some nanowires showed pure metallic behavior. Transistor like devices showed Coulomb blockade behavior at RT. The study shows that self-assembled DNA structures can be used for nanoelectronic patterning and single electron devices.

CPP 56: Focus: Computational Methods for the Energy Transition: Paving the Road to Future Materials and Storage Systems - organized by Stephan Kramer and Jochen Zausch

Time: Thursday 15:00–18:00 Location: H14

Invited Talk CPP 56.1 Thu 15:00 H14

Microstructure resolved simulations and theory based modeling: Tools for exploring the inner life of a battery — •Arnulf Latz — DLR at Helmholtz Institute Ulm for Electrochemical Energy Storage, Germany

Theory, Modeling and Simulation are important tools for creating insights in electrochemical processes from the atomistic scale to the scale of electrochemical devices. They also form the base for a future knowledge based and theory driven development of better electrochemical storage systems. Spatially resolved simulations on electrode scale can help to create a more intuitive picture of transport processes and degradation phenomena in batteries. Despite the impressive increase of in situ and operando techniques, there are still local phenomena in batteries which cannot be explored experimentally. Simulations can supplement this lack of information, if it is ensured that they can capture the spatio-temporal phenomena caused by the highly nonlinearly coupled electrochemical, multi-physics processes in batteries. This can be achieved by using as much as possible rigorous theoretical methods to derive coupled transport- electrochemistry models from fundamental principles, which try to minimize purely phenomenological assumptions. In the presentation, the development of advanced theories for electrolytes is demonstrated for the examples of solid electrolytes and ionic liquids. The impact of morphological defects and grain boundaries in all solid state batteries as well as binder distributions on the capacity, impedance and degradation of batteries is discussed with the help of pore resolved simulations.

CPP 56.2 Thu 15:30 H14

Optimizing the performance of batteries using digital material engineering — •Ilona Glatt, Fabian Biebl, Christian Wagner, and Andreas Wiegmann — Math2Market GmbH, Kaiserslautern, Germany

Key challenges to transform renewable energies into a reliable energy supply lie in optimizing its storage through increased performance of batteries. The battery performance is strongly influenced by the microstructure of the battery materials. Thus, engineering better batteries depends on understanding the impact of the micro-structure on material properties. Here, we use the simulation software GeoDict to show such an optimization on a cathode, containing a blend of the active materials Lithium Nickel Cobalt Aluminum Oxide (NCA) and Lithium Cobalt Oxide (LCO). The starting point for the optimization is a 3d-scan of the NCA-LCO cathode. Using the import module of GeoDict, the structure is segmented into three materials: electrolyte, binder and active material. The two active materials cannot be discerned based on gray values alone. In a next step, the GrainFind module is used to assign each grain to be NCA or LCO based on its shape. The result is a fully segmented cathode material containing electrolyte, binder, NCA, and LCO. Next, we use GeoDict to run a battery charging simulation and to compute other important material properties such as pore-sizes, diffusivity, conductivity, tortuosity, and mechanical properties for this cathode. Finally, we focus on finding the optimal amount of binder in the cathode by varying its amount and running geometrical analyses and a charging simulation on the resulting structure.

Invited Talk CPP 56.3 Thu 15:45 H14

Increasing the rate capability of thick graphite electrodes: Insights from MRI, NMR and porous electrode theory modelling — •Jamie Foster — University of Portsmouth, Portsmouth, UK

Utilization of thicker electrodes is one route towards improving the energy density of Li-ion batteries because it decreases the number of electrodes per cell, thereby increasing the ratio of active material to current collectors. However, the increased thickness means that it is difficult to achieve sufficiently fast transport of the lithium to supply the deep regions of the electrode with reactant. At even moderate (dis)charge rates, thick electrodes exhibit significant polarization and undesirable under-utilization of capacity.

We report experimentally determined lithium concentration profiles in a 300 micron thick graphite electrode under operation. The observed behavior clearly shows the phase transforms that are known to occur within graphite during (de)lithiation; there are sharp boundaries between graphite areas lithiated to different stages. Comparison with porous electrode theory modelling reveals that a portion of the Li is temporarily stored in the electrode surface film prior to intercalation. Although it is often difficult to fully lithiate the thick electrode, we demonstrate that the inclusion of a short current reversal, facilitates more complete lithiation. We also demonstrate the value of this high-fidelity experimental data to the modelling community, by showing how it can be used for high-confidence parameter estimation when combined with inverse modelling techniques.

CPP 56.4 Thu 16:15 H14

Combining physical and network modeling for the simulation of lithium ion batteries — •Dion Wilde and Jochen Zausch — Fraunhofer-Institute for Applied Mathematics, Kaiserslautern, Germany

For battery development numerical simulation methods can help to optimize and understand cell properties or to investigate degradation behavior. In this context physical continuum models play an important role. The drawback of these models is that the numerical solutions of the partial differential equations require significant computational effort. In applications an electrical equivalent circuit model (ECM) is often sufficient to describe the effects of interest and can be solved more efficiently. However, the parameterization of such models typically require parameter fitting since the input parameters don't have direct physical meaning. In our approach we combine a physically correct electrochemical model and the computationally fast equivalent-circuit model to formulate a physics-based equivalent circuit model which is directly linked to electrochemical parameters. The ECM is derived from the Newman model containing an element modeling the Butler-Volmer equation as well as a state-of-charge dependent voltage source representing the OCV of the designed material and resistors for electron/ion diffusion in the solid/electrolyte. Also the extension to electrochemical impedance spectroscopy is straight-forward. The system is solved by the mesh current method in python. In this contribution we will present our physical and ECM models and present a comparison between the two approaches.

15 min. break

Invited Talk CPP 56.5 Thu 16:45 H14

Numerical Simulation and Machine Learning in Virtual Materials Design — •Jan Hamaekers — Fraunhofer Institute for Algorithms and Scientific Computing SCAI, Sankt Augustin, Germany

An essential basis for designing novel materials is the understanding of their properties on the nanoscale and their effects on the macroscale. Besides theory, experiment and measurement, computational science established themselves as a new field in research and development over the last decades. In particular multiscale modeling and efficient numerical simulation techniques are powerful tools in the framework of materials design. The large amount of newly generated data from experiments and simulations together with new techniques of data analysis and machine learning have recently opened the new promising field of data-driven research. In this talk we will give on overview on selected topics in computational and data-driven science and on our recent research results and software tools.

CPP 56.6 Thu 17:15 H14

Simulating Curved Graphene Supercapacitors — •Jannes Seebeck[1] and Robert Meissner[1,2] — [1]Hamburg University of Technology, Institute of Polymer and Composites, Hamburg, Germany — [2]MagIC Magnesium Innovation Centre, Institute of Materials Research, Helmholtz Zentrum Geesthacht, Geesthacht, Germany

Supercapacitors are promising storage devices for electrical energy that offers a high power density but typically low energy density. Their storage performance is due to a reversible ion absorption by forming an electric double layer on the electrode surface. Molecular dynamics (MD) simulations offer the possibility to gain insights into the molecular mechanisms of forming electric double layers and pore filling. However, simulations show that in supercapacitors with an ionic liquid as electrolyte, the mean-field approach for calculating the differential capacitance leads to false results due to the strong correlation of ions. By using a free energy approach for the calculation of the differential capacity from the fluctuating charge density on the electrode surfaces it is possible to show a non-linear behaviour of the ionic liquid on the capacitance. Furthermore, MD-Simulations show a different orientation of the ionic liquid to the electrode interface depending on the applied potential, which can be a reason for the fluctuation of the capacity. By simulating curved graphitic electrodes, with a convex and concave pore-like structure, in combination with a diluted ionic liquid as electrolyte it is possible to examine the impact of curvature on the orientation of the ionic liquid, and finally the resulting capacity.

CPP 56.7 Thu 17:30 H14

Computational Analysis of Composition-Structure-Property-Relationships in NZP-type Materials for Li-Ion Batteries — •Daniel Mutter[1,2], Daniel F. Urban[1], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg — [2]Freiburger Materialforschungszentrum FMF, Stefan-Meier-Str. 21, 79104 Freiburg

Compounds crystallizing in the structure of $NaZr_2(PO_4)_3$ (NZP) are considered as promising materials for solid state electrolytes in Li-ion batteries. Using density functional theory (DFT), a systematic computational screening of 18 NZP compounds, namely $LiX_2(LO_4)_3$ with X = Ti, V, Fe, Zr, Nb, Ru, Hf, Ta, Os, and L = P, Mn is performed with respect to their activation energies for vacancy-mediated Li migration. It is shown how the different ionic radii of the cationic substitutions influence structural characteristics such as the octahedron volumes around Li ions on the initial and transition state sites, which affect the activation energies ("composition-structure-property"-relationships). The prevalent assumption that structural bottlenecks formed by triangularly arranged oxygen atoms at a certain location along the migration path determine the energy barriers for Li migration is not supported by the DFT results. Instead, the ionic neighborhood of the migrating ion in the initial and in the transition state need to be taken into consideration to relate the structure to the activation energies. This conclusion applies to Na containing NZP compounds as well.

CPP 56.8 Thu 17:45 H14

The origin of unstable sodium graphite intercalation compounds — Olena Lenchuk and •Doreen Mollenhauer — Institute of Physical Chemistry, Justus-Liebig University Giessen, Heinrich-Buff-Ring 17, D-35392 Giessen, Germany

First principles investigations can contribute to the understanding of intercalation mechanisms and compounds chemistry important for supporting the development of battery materials such as sodium-ion batteries (SIBs).[1] The commonly used negative electrode graphite for lithium-ion batteries does not intercalate sodium ions in high concentrations [2,3] whereas intercalation of potassium is possible. In order to understand the origin of Na-GICs (binary graphite intercalation compounds) instability compared to stable Li- and K-GIC we performed dispersion corrected density-functional theory (DFT) calculations. We analyzed and compared in detail the interplay between the structural deformation and binding contributions of the different alkali metal-GIC. This allows us to identify main factors for the instability of Na-GICs [4].

[1] M. Goktas, C. Bolli, E. J. Berg, P. Novak, K. Pollok, F. Langenhorst, M. v. Roeder, O. Lenchuk, D. Mollenhauer, P. Adelhelm, Adv. Energy Mater. 2018, 1702724. [2] K. Nobuhara, H. Nakayama, M. Nose, Sh. Nakanishi and H. Iba, J. Power Sources 243 (2013) 585-587. [3] Zh. Wang, S.M. Selbach and T. Grande, RSC Adv. 4 (2014) 4069-4079. [4] O. Lenchuk, P. Adelhelm, D. Mollenhauer, Manuscript to be submitted.

CPP 57: Organic Electronics and Photovoltaics IV - Excitonic Properties and Light-Emitting Devices

Time: Thursday 15:00–18:15 Location: H18

CPP 57.1 Thu 15:00 H18

Optical Probing of the Various Operation Regimes in Organic Light-Emitting Diodes Using Molecular Probes — •Thomas Ferschke[1], Alexander Hofmann[2], Wolfgang Brütting[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, Julius Maximilian University, 97074 Würzburg — [2]Institute of Physics, University of Augsburg, 86135 Augsburg — [3]ZAE Bayern, 97074 Würzburg

Photoluminescence (PL) studies on single guest molecules have been shown to enable determination of charge carrier distribution in organic opto-electronic devices on nanometer length scales.[1] In this work, this principle is adapted to the various operation regimes of Alq$_3$/α-NPD OLEDs. Tetraphenyldibenzoperiflanthene (DBP) dopants are incorporated at distinct vertical positions within the active layers of the OLED stack. Measuring the DBP optical properties under different operation conditions of the device, the significant reduction in PL upon charge carrier injection (forward bias regime) can be attributed to non-radiative decay channels promoted by the exciton-electron interaction. Studying this effect as function of current density and dopant position reveals information on the local charge carrier distribution. Under reverse bias, a strong PL quenching of DBP probes in close proximity to the Alq$_3$/α-NPD interface is observed as well. This can be related to the strong electric fields caused by Alq$_3$ charges localized at the interface.[2] We substantiate this hypothesis by complementary data obtained by impedance spectroscopy on the identical OLED devices.

[1] Nothaft *et al.*, *ChemPhysChem*, **2011**, 12, 2590–2595

[2] Noguchi *et al.*, *J. Appl. Phys.*, **2012**, 111(11):114508

CPP 57.2 Thu 15:15 H18

Temperature (De-)Activation in Donor-Acceptor based Organic Light Emitting Diodes — •Sebastian Weissenseel, Felix Klingert, Jeannine Grüne, Nikolai Bunzmann, Andreas Sperlich, and Vladimir Dyakonov — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

The world of organic light emitting diodes (OLEDs) regained a lot of attention with the publication of Goushi et al. in 2012 [1], where the thermal activation of non-radiative triplets via reverse intersystem crossing (RISC) was applied to enhance the fluorescence in OLEDs for the first time. Here, we investigate the donor-acceptor based system 4,4',4"-Tris(N-3-methylphenyl-N-phenyl-amino)triphenylamine (m-MTDATA): Tris(2,4,6-trimethyl-3-(pyridin-3-yl)phenyl)borane (3TPYMB), which exhibits an intermolecular TADF mechanism. The devices are analyzed by means of temperature dependent current-electroluminescence-voltage (j-EL-V) characteristics and external quantum efficiency (EQE). These measurements were intended to estimate the activation energy of the triplet-to-singlet upconversion and thus the singlet-triplet gap. Surprisingly, we observe typical TADF-like efficiency enhancement with rising temperature only in a limited temperature range 180-250K, while at higher temperature (>250K), this trend inverts and we observe a decrease in EQE. This observation implies the competing process between thermally activated RISC and a non-radiative decay at ambient temperature in TADF OLEDs, which is essential for their further improvement.

[1] Goushi, et al., Nat. Photon. **6**, 253 (2012)

CPP 57.3 Thu 15:30 H18

Time-resolved Spectroscopy of Organic Light Emitting Diodes based on Thermally Activated Delayed Fluorescence — •Jeannine Grüne, Nikolai Bunzmann, Sebastian Weissenseel, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Organic light emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF) show increased efficiencies due to efficient upconversion from the non-emissive triplet states to the emissive singlet state via reverse intersystem crossing (RISC). Therefor a small energetic splitting between singlet and triplet states is required which can be achieved by formation of an exciplex state, a weakly bound electron-hole pair at a donor:acceptor interface. A proven material combination is among others 4,4',4"-Tris[(3-methylphenyl)phenylamino]triphenylamine (m-MTDATA), as donor and Tris(2,4,6-trimethyl-3-(pyridin-3-yl)phenyl)borane (3TPYMB), as acceptor. We investigated this system with time-resolved electroluminescence (trEL) in combination with time-resolved magnetic resonance techniques based on EL and photoluminescence detection (trELDMR, trPLDMR). In the latter case, microwave irradiation is used to induce transitions between the triplet states which are split in a present magnetic field. By applying microwave pulses over several microseconds, the spin-dependent EL modulation processes as well as the corresponding time frames can be identified, to get a better understanding of the triplet contribution to the TADF mechanism.

CPP 57.4 Thu 15:45 H18

A refined setup for an enhanced signal-to-noise ratio in angular resolved photoluminescence measurements — •Christian Hänisch, Simone Lenk, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, 01187 Dresden, Germany

Controlling the orientation distribution of transition dipole moments in the emission layer of organic light-emitting diodes is one of the key approaches for further enhancements of the device efficiencies. In order to investigate this physical parameter typically angular resolved photoluminescence measurements are performed.

In this contribution, we present an advanced concept which adds two plano-convex lenses to the conventional measurement setup in order to collect and focus the initially emitted light to the detector fiber. In this manner, the signal-to-noise ratio of the recorded emission spectra can be drastically improved, which enables measurements of weakly emitting or fast degrading material systems.

A detailed ray transfer analysis is performed, which on the one hand reveals the required parameters of the optical components and on the other hand allows for a detailed evaluation and optimization of the setup alignment.

CPP 57.5 Thu 16:00 H18

Kinetic Modelling of Transient Photoluminescence from Thermally Activated Delayed Fluorescence — •Nils Haase[1,2], Andrew Danos[3], Christof Pflumm[2], Antonia Morherr[2], Patrycja Stachelek[3], Amel Mekic[2,4], Wolfgang Brütting[1], and Andrew P. Monkman[3] — [1]University of Augsburg, Augsburg, Germany — [2]Merck KGaA, Darmstadt, Germany — [3]Durham University, Durham, UK — [4]University of Regensburg, Regensburg, Germany

Thermally activated delayed fluorescence (TADF) is an established mechanism for harvesting triplet excitons in *metal-free* OLEDs [1] which gives a maximum attainable internal quantum efficiency of 100%. By minimizing the energy gap between the lowest lying singlet and triplet states, a conversion of slowly relaxing triplet sates to faster relaxing singlet states via reverse intersystem crossing rate (rISC) is promoted. Although several highly efficient TADF emitters have been discovered, a reliable determination of the reverse intersystem crossing rate as a key parameter for the characterization of TADFs has not been provided yet. In this work, we present a kinetic model for the TADF process which allows to extract not only rate constants but also time dependent state populations from transient photolumines-cence experiments. Using this model, we obtain temperature dependent rISC rates from which we calculate the activation energy for the TADF process.

[1] Uoyama et al., Nature 492 (2012), 234*238.

CPP 57.6 Thu 16:15 H18

Detecting magnetic resonance in Earth's magnetic field — •Sebastian Milster, Tobias Grünbaum, Simon Kurrmann, Hermann Kraus, Sebastian Bange, and John M. Lupton — Universität Regensburg,Institut für Experimentelle und Angewandte Physik, Universitätsstraße 31, 93053 Regensburg, Germany

Electron paramagnetic resonance in OLEDs [1] at magnetic field strengths comparable to Earth's field offers a way to model the migratory orientation ability of some birds [2] to a certain extent in a laboratory setting.

With the expected resonance position at a field of approximately 44 microtesla for a frequency of 1.315 MHz [3], even small stray fields as well as Earth's magnetic field have a rather large effect and create a shift on the magnetic field axis, depending on their orientation to the external applied field. As a consequence, the expected resonance peaks partially overlap with other effects in the device, thus becoming almost unresolvable. By compensating all parasitic fields with a three-dimensional arrangement of Helmholtz coils, it is possible to nullify the shifting effects. Following this, the resonances become resolvable for frequencies even in the low MHz-regime. By optimizing the experimental parameters preliminary results are presented, showing EPR at a frequency of 1.315 MHz, in resonance with the Zeeman splitting induced by Earth's field.

[1] H. Kraus et al., Phys. Rev. B 95, 241201(R)(2017)
[2] W. Wiltschko et al., Science 176, 71-77 (1972)
[3] W. Baker et al., Nat. Commun. 3, 898 (2012)

15 min. break

CPP 57.7 Thu 16:45 H18

Spectroscopic study of a novel iron based charge-transfer complex — •Nils W. Rosemann[1], Kasper Skov Kjaer[1], Nidhi Kaaul[2], Om Prakash[3], Pavel Chábera[1], Alireza Honarfar[1], Olga Gordivska[3], Lisa A. Fredin[4], Karl-Erik Bergquist[3], Lennart Häggström[5], Tore Ericsson[5], Linnea Lindh[1], Arkady Yartsev[1], Stenbjörn Styring[2], Ping Huang[2], Jens Uhlig[1], Jesper Bendix[6], Daniel Strand[3], Villy Sundström[1], Petter Persson[4], Reiner Lomoth[2], and Kenneth Wärnmark[3] — [1]Division of Chemical Physics, Department of Chemistry, Lund University, Sweden — [2]Department of Chemistry - Ångström Laboratory, Uppsala University, Sweden — [3]Center for Analysis and Synthesis, Department of Chemistry, Lund University, Sweden — [4]Division of Theoretical Chemistry, Department of Chemistry, Lund University, Sweden — [5]Department of Physics and Astronomy - Ångström Laboratory, Uppsala University, Sweden — [6]Department of Chemistry, University of Copenhagen, Denmark

Complex molecules based on transition metals are used in solar light harvesting, e.g., dye-sensitized solar cells and photocatalysis. Standard complexes are based on scarce metals like ruthenium. This calls for replacements based on abundant metals like, e.g., Iron (Fe). Here, we present our latest results on a Fe-based complex. By coordination of two tris-carbene ligands to the Fe centre in an octahedral geometry the deactivation through metal centred states is drastically suppressed. Thus, unmatched 2 ns room temperature excited state lifetime and 2% photoluminescence quantum yield are achieved.

CPP 57.8 Thu 17:00 H18

Coherent dynamics of ultrafast singlet fission in Pentacene — •Ajay Jha[1], Hong-Guang Duan[1,2,3], Xin Li[4], Vandana Tiwari[1], Hanyang Ye[5], Pabitra Nayak[5], Xiao-Lei Zhu[4], Zheng Li[1], Todd Martinez[4], Michael Thorwart[2,3], and R. J. Dwayne Miller[1,3,6] — [1]MPSD, Hamburg, Germany — [2]I. Institut für Theoretische Physik, UH, Germany — [3]CUI, Hamburg, Germany — [4]Stanford University, US — [5]University of Oxford, UK — [6]University of Toronto, Canada

Singlet fission is one of the possible ways to circumvent the Shockley-Queisser limit on efficiency. Pentacene and its derivatives have shown great promise towards their application in devices to harness photons for carrier multiplication via singlet fission process. Here we study the singlet fission process in a pentacene thin film using a combination of transient-grating and two-dimensional electronic spectroscopy complemented by quantum chemical and nonadiabatic dynamics calculations. Our study reveals that along with the high-frequency vibrations, intermolecular rocking motions drive the ultrafast dynamics at the multidimensional conical intersection in the singlet fission process.

CPP 57.9 Thu 17:15 H18

Molecular Structure and Geometry Packing Effects on Singlet Fission Mechanism — •N. Alagna[1], J. Han[2], N. Wollscheid[1], J.L. Perez Lustres[1], J. Herz[1], S. Hahn[3], S. Koser[3], F. Paulus[3], U. Bunz[3], A. Dreuw[2], T. Buckup[1], and M. Motzkus[1] — [1]Physikalisch- Chemisches Institut, Ruprecht- Karls-Universität Heidelber — [2]Institut für Wissenschaftliches Rechnen, Ruprecht-Karls Universität Heidelberg — [3]Organisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg

Efficiency limit of organic photovoltaic can be overcome by singlet fission (SF), a photo induced processes where two triplet states are formed from an excited singlet state. Molecular structure and packing arrangement are critical for SF. In this work, quantum chemistry, organic synthesis and time resolved spectroscopy are applied to rationalize how SF is effected by systematic chemical modification induced in phenazinothiadiazoles (PTD). Substitution of an aromatic ring of TIPS-Tetracene by a thiadiazole group change in a considerable way the relative energy of S1 and T1 states. In contrast with TIPS-tetracene, SF became exothermic for PTD derivatives, which show an energy difference S1-2T1 higher of 0.44 eV. This enables SF in PTD derivatives, where the fs formation of the T-T state is identified by transient absorption spectroscopy and TD-DFT calculation. Moreover, we show via CDFT-CL calculations that dimer architecture control the strength and coaction between direct and superexchange couplings, that accelerate the SF rate constant beyond 100 fs.

CPP 57.10 Thu 17:30 H18

Investigating diffusion controlled singlet fission of a chlorinated phenazinothiadiazole. — •Nikolaus Wollscheid[1,3], Nicolo Alagna[1], José Luis Perez Lustres[1,3], Victor Brosius[2], Florian Geyer[2], Uwe Bunz[2,3], Tiago Buckup[1], and Marcus Motzkus[1,3] — [1]Physikalisch- Chemisches Institut, Ruprecht- Karls-Universität Heidelberg — [2]Organisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg — [3]Centre for Advanced Materials, Ruprecht-Karls-Universität Heidelberg

Singlet fission (SF) is a carrier multiplication process where one excited singlet state yields two triplet states upon close interaction of two chromophores. This ultrafast photoreaction was first observed in solid state and has strong implications in organic photovoltaics. In order to disentangle the mechanism by extending the dynamics to longer timescales, concentrated solutions of TIPS-Tetracene were investigated. Here, the reaction is controlled by the diffusion of the reaction partners, which allowed for the isolation of the spectrum of an intermediate excimer state [1]. In this work, we use ultrafast transient absorption spectroscopy to investigate concentrated solutions of a chlorinated phenazinothiadiazole in toluene. The observation of a correlation between singlet decay and triplet formation, combined with the linear dependence of the corresponding decay rate on concentration, indicates diffusion controlled SF. For high concentrations, spectral analysis suggests direct and efficient SF, whereas an additional process is observed for low concentrations.

[1] H. L. Stern *et al.*, *PNAS*, **112**, 7656 (2015).

CPP 57.11 Thu 17:45 H18

Homocoupling defects limit exciton diffusion in a conjugated polymer — •Martin Streiter[1], Fabian Meier[1], Daniel Beer[1], Caroline Lienert[2], Florian Lombeck[2], Michael Sommer[2], and Carsten Deibel[1] — [1]Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany — [2]Institut für Makromolekulare Chemie, Universität Freiburg, 79104 Freiburg, Germany

Exciton diffusion has been studied in a range of conjugated polymers. It is both, of fundamental interest and an important step relevant for high performance organic solar cells. Copolymers such as PCDTBT are commonly employed as donor material in bulk heterojunction solar cells. Recently, chemical defects such as homocouplings have been shown to form at the material synthesis stage, severely limiting the short circuit current of organic photovoltaics. Here we show that indeed carbazole homocoupling limits exciton diffusion in PCDTBT. We propose a mechanism that explains the limitation of exciton diffusion caused by high homocoupling concentrations and short chain lengths. Diffusion is limited when either chain length or homocouplings impair the effective conjugation length of the polymer chain.

CPP 57.12 Thu 18:00 H18

Correlated Atomic Force Microscopy and Spatially-resolved Photoluminescence Spectroscopy Study of Merocyanine Aggregate Thin Films — •Lukas Böhner, Thorsten Limböck, Dirk Hertel, Klas Lindfors, and Klaus Meerholz — University of Cologne, Köln

Merocyanine molecules are interesting materials for organic solar cells (OSCs) due to their high absorption coefficients [1]. Large area OSCs can be produced at low cost. However, the in this way resulting disordered structure of the active material in OSCs is disadvantageous in terms of exciton- and charge mobility. One strategy to increase order in organic materials is the utilization of molecular aggregates wherein excitons are delocalized. Additionally aggregation of organic dye molecules leads to drastic changes of the optical properties compared to the monomeric form [2]. Here, we study thin films of merocyanine molecular aggregates fabricated by vacuum deposition. The morphology of the films is varied by using different substrates and controlling the deposition parameters. Combining atomic force microscopy and photoluminescence microspectroscopy we are able to correlate the structural and optical properties of the aggregates. We find that by suitable choice of the fabrication parameters, thin films consisting of crystalline domains which scale in the range of tens of micrometers can be obtained. We will present the impact of molecular order on exciton and charge transport properties. References: [1] H. Bürckstümmer, et al., Angew. Chemie - Int. Ed. 2011, 50, 11628-11632. [2] A. Liess, et al., Adv. Funct. Mater. 2018, 1805058, 1-9.

CPP 58: Nanostructures, Nanostructuring and Nanosized Soft Matter

Time: Thursday 15:00–18:30 Location: H13

Invited Talk CPP 58.1 Thu 15:00 H13

Gyroids on the nanoscale: Metamaterials with surprising optical properties — •Bodo Wilts — Adolphe Merkle Institute, University of Fribourg, Fribourg, Switzerland

Block copolymers can self-assemble into various nanostructured morphologies, such as lamellae, cylinders, spheres and the gyroid. Such polymeric structures can be used as templates to fabricate functional nanostructured materials. This bottom-up fabrication route allows generating materials with different, or entirely novel, properties. One example are optical metamaterials, metallic structures with unit cells smaller than the wavelength of light. Here, I will show that optical metamaterials can be fabricated by replicating gyroid polymeric nanostructures into plasmonic metals. The cubic gyroid structure is of particular interest for optical metamaterials applications due to its inherent chirality, which promises to induce novel optical properties in gyroid metal replica. I will demonstrate that these gyroids indeed show surprising optical properties such as linear and circular dichroism, and will show that these properties originate from a contribution of the surface morphology and the local orientation of the gyroid structure. I will discuss the importance of structural order of the polymeric templates on the resulting optical metamaterials and will further outline how changing the material composition, e.g. by changing the material from gold to silver, changes the optical properties of the nanostructures.

CPP 58.2 Thu 15:30 H13

The real 3D morphology of cylindrical block copolymer nanomasks — •Daniel Kool[1,2], Katharina Brassat[1,2], and Jörg K. N. Lindner[1,2] — [1]University of Paderborn, Dept. of physics, Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn CeOPP, Paderborn, Germany

Block copolymer (BCP) lithography is a well-established technique which allows for economical large-area patterning of surfaces with self-assembled nanoscale features. We exploit the microphase separation of copolymers, here poly(styrene-b-methyl methacrylate) (PS-b-PMMA) BCP with a block length ratio of 70:30. This results in the formation of 17 nm diameter PMMA cylinders perpendicular to the surface and hexagonally arranged in a PS matrix. After selective removal of PMMA cylinders the nanostructured PS thin film can be used in common lithography processing steps, as reactive ion etching and lift-off for pattern replication and transfer. Here we demonstrate that the efficiency of replication of the nanostructured features can be drastically improved by modification of the polymer mask prior to lithographic use by an O_2 plasma treatment. We achieved an experimental method of pattern replication without loss of features and the opportunity to tune the feature size precisely on the nanometer scale. By SEM investigations of both interfaces of the lithography mask we were able to reconstruct the 3-dimensional morphology of the polymer mask. Indirect information on the polymer mask morphology is obtained, in addition, from pattern replication studies by lift-off experiments and by RIE, allows to conclude on the real 3D shape of BCP pores.

CPP 58.3 Thu 15:45 H13

Research of the high loading capacities of amphiphilic Poly(2-Oxazoline)-based Triblockcopolymers with Curcumin — •Özgür Düdükcü[1], B. Sochor[1], M. Lübtow[3], B. Schummer[1,2], R. Luxenhofer[3], and R. Hanke[1,2] — [1]Institute of Physics, Chair of X-ray Microscopy, Universität Würzburg, Germany — [2]Fraunhofer Insitiute for Integrated Circuits IIS, Development Center X-ray Technology EZRT, Fürth, Germany — [3]Functional Polymer Materials, Chair for Advanced Materials Synthesis, Department of Chemistry and Pharmacy and Bavarian Polymer Institute, Universität Würzburg, Germany

In this project, drug-loaded triblock copolymers in solu- tions were investigated using small-angle-neutron-scatter- ing (SANS), densiometric measurements and 1H-NMR Spectro- scopy. Curcumin was used as the hydrophobic drug and Poly (2-Oxazoline)-based amphiphilic triblock copolymers as carrier systems. The triblock copolymers consist of a hydrophobic middle block and hydrophilic side chains. Polymer carrier systems in nanomedicine typically have loading capacities of less than 10-20 %. The aim of the project was to clarify the high drug loading capacities up to 80 wt% of the investigated formulations. This effect is still unexplained. By analysing the scattering curves of the formulations resulting from the SANS experiments, information about the structure and composition of the formulations was obtained. The scattering curves are compared with theoretical models to clarify the structure of formulated drug-polymer-systems. The analysis showed that the drug-loaded polymers form micelles with a hydrophobic core and two outer shells, i.e. a core-shell-shell model. Including 1H-NMR measurements it was found that curcumin does not only accumulate in the hydrophobic core. Despite its hydrophobic character interacts with the hydrophilic side chains of the triblock copolymer and forms a second shell. Thus this model gives a possible explanation of the high loading capacity of the polymers.

CPP 58.4 Thu 16:00 H13

Sputter deposition of Al on nanostructured PMMA-b-P3HT and PS-b-PMMA copolymer thin films — •Marc Gensch[1,2], Matthias Schwartzkopf[1], Jonas Drewes[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Franz Faupel[3], Peter Müller-Buschbaum[2], and Stephan Volkher Roth[1,4] — [1]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, D-22607 Hamburg, Germany — [2]Technische Universität München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, D-85748 Garching, Germany — [3]Lehrstuhl für Materialverbunde, Institut für Materialwissenschaft, Christian Albrechts-Universität zu Kiel, Kaiserstr.2, D-24143 Kiel, Germany — [4]KTH Royal Institute of Technology, Teknikringen 56-58, SE-100 44 Stockholm

Nanostructured polymer-metal-composite films show great perspectives for optoelectronic applications, e.g. as sensors or photovoltaics. To tailor properties of such devices the self-assembly process of the nanostructures needs to be understood. We studied in situ the evolution of the cluster growth morphology by grazing incidence small-angle X-ray scattering (GISAXS), the crystallinity of the nanogranular metal film with grazing incidence wide-angle X-ray scattering (GIWAXS) and the optical properties using surface differential reflectance spectroscopy (SDRS) all simultaneously during Al sputter deposition on nanostructured polymer templates. Our study reveals the selective decoration of Al on the polymer domains and the templates influence on the percolation behavior of the Al layer.

CPP 58.5 Thu 16:15 H13

Pattern transfer of self-assembled block copolymer nanopores into silicon and silicon dioxide by reactive ion etching — •Alexander Stratmann, Daniel Kool, Julius Bürger, Katharina Brassat, and Jörg K. N. Lindner — Paderborn University, Paderborn, Germany

Reactive ion etching (RIE) is a highly reproducible dry etching method, which combines the benefits of physical sputtering with ions and chemical etching with radicals. By combining RIE processes with block copolymer (BCP) lithography large-area nanopore patterns in the sub-20 nm regime can be created. To this end, the self-ordering of a polystyrene-*b*-methyl methacrylate (PS-*b*-PMMA) BCP is exploited to create hexagonally arranged PMMA cylinders in a PS matrix. After the selective removal of the PMMA cylinders the PS thin film can be used for common lithography processes such as RIE. The pattern transfer was accomplished on silicon and silicon dioxide surfaces by etching with a SF_6/Ar and a CHF_3/Ar plasma, respectively. To complete the lithography process, the removal of the mask was done by an O_2/Ar plasma. We achieved a highly reproducible method to etch nanopores with homogenous etching depth, etch profile, pore diameter and high feature density. The process steps are investigated by SEM, AFM and cross-sectional TEM.

15 min. break

CPP 58.6 Thu 16:45 H13

Dye-Sensitized Ternary Copper Chalcogenide Nanocrystals: Optoelectronic Properties, Air Stability and Photosensitivity — •Sonam Maiti[1,2], Santanu Maiti[2], Ali Hossain Khan[3], Frank Schreiber[2], and Marcus Scheele[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen, Germany. — [2]Institute of Applied Physics, University of Tubingen, Germany — [3]Department of Chemistry, Ghent University, Belgium

Copper chalcogenide nanocrystals (NCs) exhibit a great potential for optoelectronic applications and efforts have been made to increase electronic coupling in thin films of these materials.1-2 We report on the effect of ligand exchange of Cu2-xSeyS1-y as well as Cu2-xSe nanocrystals (NCs) with the organic pi-system Cobalt β-tetraaminophthalocyanine (CoTAPc) and analyze changes in the structural, optical as well as electronic properties. A strong ligand interaction with the surface of the NCs is revealed by absorption and Raman spectroscopy. Grazing-incidence small-angle X-ray scattering studies show a significant contraction in the interparticle distance upon ligand exchange. For Cu2-xSe, this contraction has a negligible effect on electric transport, while for Cu2-xSeyS1-y the conductivity increases by eight orders of magnitude and results in metal-like temperature-dependent transport. With photocurrent measurements, we demonstrate high optical responsivities for Cu2-xSeyS1-y NCs and show the organic pi-system acts as an electronic linker and an optical sensitizer at the same time. 1. C. Coughlan et al, Chem Rev 2017, 117 (9), 5865-6109. 2. S. Maiti et al, JPCC 2018, 122 (41), 23720-23727.

CPP 58.7 Thu 17:00 H13

Following the formation of metal electrodes on photoactive polymer thin films — •Franziska Löhrer[1], Volker Körstgens[1], Simon Schaper[1], Matthias Schwartzkopff[2], Alexander Hinz[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Franz Faupel[3], Stephan Roth[2,4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, D-85748 Garching — [2]Deutsches Elektronensynchrotron DESY, D-22607 Hamburg — [3]CAU zu Kiel, Institut für Materialwissenschaft, D-24143 Kiel — [4]KTH, Teknikringen 56-58, SE-100 44 Stockholm

Although based on organic materials, organic solar cells often include metal electrodes due to their unrivaled electronic conductivity. Thus, polymer-metal interfaces are inherently present in most OPV devices and have a major influence on their behavior. Understanding the growth mechanisms of metal contacts on polymer thin films plays a crucial role in identifying potential ways to enhance the device performance. We investigate the morphological changes at the metal-polymer interface during the sputter deposition of metal contacts onto photoactive polymer films via in-situ GISAXS. This technique allows insights into the structural evolution of the metal on the organic film. A model describing the process is developed based on earlier work on different material systems. Comparing the deposition behavior of typical electrode materials on thin films of photoactive organic materials helps to understand their influence on the respective device performance.

CPP 58.8 Thu 17:15 H13

Structural and melting properties of low molecular weight PEG confined in nanoporous ITPC — •Ann-Kathrin Grefe, Björn Kuttich, and Bernd Stühn — Institut für Festkörperphysik, Technische Universität Darmstadt

Ion track-etched polycarbonate constitutes an ideal system for studying confined polymers. Whereas other nanoporous systems often rule out small angle x-ray scattering due to predominant pore scattering and laborious data description, ITPC allows for a more straightforward investigation since the pores are not structurally correlated.[1]

Nanopores with radii from 8 to 205 nm are prepared and coated with 10 nm of SiO_2 via ALD in order to obtain a well-defined and homogeneous surface. SAXS reveals the nearly perfect cylindrical geometry of the pores. The linear dependency of the pore radius on the etching time is shown to hold true over the complete range of pore radii.

PEG with $M_w = 1500\,\mathrm{g/mol}$ and a semicrystalline lamellar bulk structure is introduced into the nanopores via melt infiltration. At high temperatures SAXS confirms a nearly complete filling with amorphous polymer. Upon cooling below the melting point of PEG, a concentrical arrangement of semicrystalline lamellae is revealed for pore radii over 71 nm. We introduce models which successfully describe the combined scattering from nanopores and semicrystalline or amorphous PEG inside. DSC measurements of the confined polymer show a decrease of melting temperature and heat of fusion per gram polymer upon reduction of the pore radius and hint at a change in nucleation mechanism.

[1] M. Engel et al., Appl Phys A 97, 99-108 (2009)

CPP 58.9 Thu 17:30 H13

High-resolution multi-channel nanoparticle separation utilizing rocked Brownian motors — •Christian Schwemmer, Francesca Ruggeri, Xiaoyu Ma, and Armin Knoll — IBM Research - Zurich, Switzerland

Artificial Brownian motors were inspired by how nature achieves directed transport in highly diffusive environments [1]. Their two main ingredients are an asymmetric potential and a zero-mean driving force. Our implementation employs the electrostatic interactions in weak electrolytes between charged nanoparticles and like charged surfaces of a nanofluidic slit [2] to define a ratchet shaped energy landscape [3]. A zero-mean AC electric field across the slit induces an electro-osmotically transduced driving force, resulting in drift speeds of up to $50\,\mu$m/s for 60 nm gold spheres. The motors exhibit an Arrhenius-like onset of the particle current with decreasing amplitude of the energy barriers, a promising feature for particle separation [4]. Based on this property, we developed a fast and highly selective nanoparticle sorting device to separate gold spheres of nominally 80 nm and 100 nm diameter along its y-axis into 30 subpopulations with $<$2 nm sorting resolution. By switching the AC field to the x-direction, the separated populations are transported to compartments for collection. Thus, scalable continuous multi-channel particle separation is within reach.

[1] Hänggi et al., Rev. Mod. Phys., **81**, 387 (2009)
[2] Krishnan et al., Nature, **467**, 692 (2010)
[3] Skaug et al., Science, **359**, 1505 (2018)
[4] Bartussek et al., Europhs. Lett., **28**, 459 (1994)

CPP 58.10 Thu 17:45 H13

Nanoporous Gold supported Polypyrrole: Electrochemically Modulated Elasticity — •Jie Li[1], Jürgen Markmann[1,2], Jörg Weissmüller[1,2], and Nadiia Mameka[1] — [1]Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Materials Mechanics — [2]Hamburg University of Technology, Institute of Materials Physics and Technology

Polypyrrole (PPy), an intrinsic conducting polymer, has drawn widespread attention in many fields, such as, displays, ion exchange membranes and actuators, where mechanical integrity is required by functionalities. Thin films preparation and their mechanical properties, say, strength, have been widely studied, whereas the elastic modulus, especially the modulus under stress coupled with electrochemical conditions, remains to be clarified. Herein, PPy film is electropolymerized on mm-size nanoporous gold (NPG), a 3D bicountinuous network of nanoscaled ligaments and pores with large surface area [1]. Uniform PPy coatings with various thicknesses in bulk NPG are achieved without blocking the original nanopores. The elastic modulus measurements of NPG-PPy composites were performed in situ during potential cycling in aqueous electrolyte in a dynamic mechanical analyzer (DMA). In situ DMA experiments reveal a non-monotonic modulus response versus the potential during charging-discharging processes, as opposed to nearly linear variation of the macroscopic length. Moreover, the modulus variation amplitude increases with the PPy film thickness. Possible mechanisms for the stiffness behavior will be discussed. [1] Mameka et al, Mater. Res. Lett., 2016, 1:27.

CPP 58.11 Thu 18:00 H13

Structural Characteristics of Small and Stable Coenzyme Q10 Nanoparticles produced by Antisolvent Precipitation — •Isabel Schuldes, Dennis M. Noll, Tobias Zech, and Tobias Unruh — Institute for Crystallography and Structural Physics, Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany

The production of organic nanoparticles (NPs) via antisolvent precipitation (AP) is a less-invasive and low-cost alternative to top-down methods like high-pressure homogenization. Thus, AP is receiving growing attention, e.g. for the preparation of nanodispersions of pharmaceutical ingredients. For instance, the antioxidant coenzyme Q10 (Q10) has several health protective effects and Q10 NPs showed improved bioavailability compared to free Q10.

Here we report the structural characterization of Q10 NPs produced by AP. The NPs are analyzed by photon correlation spectroscopy (PCS), cryogenic transmission electron microscopy (CryoTEM), small-angle X-ray and neutron scattering (SAXS; SANS, KWS-1 at MLZ). In particular, the combination of SAXS and SANS studies allows the investigation of the molecular structure of the NPs and the interface between the NPs and the dispersion medium. Our experiments revealed, that Q10 NPs prepared by AP are stable with and without added stabilizer, have a particular small size (down to ~ 20 nm in diameter), and exhibit a specific stabilizing layer, suggesting a self-stabilizing process of the Q10 molecules.

CPP 58.12 Thu 18:15 H13

The impact of inhomogeneous distributions and magnetisation of nanoparticles on the equilibrium structure of magnetic filaments — •Deniz Mostarac[1], Pedro A. Sanchez[1,2], Oleg Gang[3,4], and Sofia Kantorovich[1,2] — [1]University of Vienna, Vienna, Austria — [2]Ural Federal University, Ekaterinburg, Russia — [3]Columbia University, New York, USA — [4]Brookhaven National Laboratory, New York, USA

Construction of smart materials with sophisticated magnetic response by incorporating magnetic particles (MNP's) within permanently cross-linked structures, opens the possibility for applications to highly magneto-responsive systems [1]. Construction of magnetic filaments (MF's polymer-like structures in which as monomers are the magnetic beads) is possible using DNA origami technique [2,3]. Structural inhomogeneities alter the equilibrium properties and the magnetic response of MF's. Using MD simulations, we show that coiling and persistence length of MF's depend on the magnetic particle distributions, along with temperature and applied magnetic field. We compare the structural properties and magnetic behaviour of different configurations of MF's, highlighting that our model takes in to account superparamagnetic effects. We present an exhaustive, comparative analysis of the field dependent, structural behaviour of MF's.

[1] Sánchez, P. A., et al. Macromolecules 48.20 (2015): 7658-7669. [2] Liu, W., et al. Nature chemistry 8.9 (2016): 867. [3] Tian, Y., et al. Nature materials 15.6 (2016): 654.

CPP 59: Composites and Functional Polymer Hybrids

Time: Thursday 15:00–17:30 Location: H8

Invited Talk CPP 59.1 Thu 15:00 H8

Polymer-Grafted Nanoparticle Membranes with Exceptional Gas Separation Performance — •Sanat Kumar — Columbia University, Department of Chemical Eng., New York, NY 10025, USA

Polymeric membranes represent an efficient solution for separating gas mixtures, e.g., for natural gas purification. Several recent reviews emphasize that improved mechanical and gas separation (i.e., increased permeability and selectivity) performance is required from next-generation constructs; achieving these goals require that predictive structure-property relationships be developed for these materials. In this vein, here we leverage our evolving understanding of polymer brush physics to systematically design membranes which show exceptional improvements over the current state-of-the-art. We show that, while pure polymer-grafted nanoparticle (GNPs) membranes yield increased gas permeability through graft density and chain length variations, mixing GNPs with ungrafted polymers improves selectivity so that we routinely outperform the best currently available polymers. Surprisingly, we find that transport in pure GNPs is spatially inhomogeneous with large gases moved primarily through interstices, while smaller solutes diffuse more homogeneously in the polymer layer. Free chains segregate into these interstices, preferentially hindering large solute motion, thus dramatically improving selectivity. The ability to exploit spatial inhomogeneities in GNPs with ungrafted chains is a new, apparently general, paradigm to design membranes with unprecedented performance even using common polymer architectures.

CPP 59.2 Thu 15:30 H8

Insights into the porous structure of metal-imidazolate frameworks having high gas uptake — •Ahmed. G. Attallah[1], Suvendu. S. Mondal[2], Hans-Jürgen Holdt[2], and Reinhard Krause-Rehberg[3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics, Bautzner Landstr. 400, 01328 Dresden, Germany — [2]Institut für Chemie, Anorganische Chemie Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [3]Institut für Physik, Martin-Luther-Universität, Von-Danckelmann-Platz 3, 06120 Halle, Germany

Several methodologies, like pore surface-amines functionalization, defect engineering, and others have been evolved to improve gas uptake by Metal-Organic-Frameworks(MOFs). It was reported that microwave(MW)-assisted synthesis of MOFs exhibited an enhancement of N2 and CO2 uptake capacity, compared to the analogous Conventional Electric(CE)-heating based materials. However, no detailed investigations on the origin of the high guest uptake capacity of MW-assisted materials have been carried out. In this work, three MW-assisted isostructural Imidazolate-Framework-Potsdam(IFP) which showed an enhancement of CO2 and H2 uptake capacities are investigated. These three samples have flexible methoxy and ethoxy linker arms. Thus, the aim here is to understand the reasons for the high gas uptake of materials synthesized by the MW-assisted conditions compared with the same materials synthesized by CE-heating methods. This study is performed by Positron Annihilation Lifetime Spectroscopy (PALS) in addition to other characterization methods.

CPP 59.3 Thu 15:45 H8

Touching and detachment: Nickel-particle movement in an elastomer matrix under exertion to magnetic field — •Henrik Schmidt[1] and Günter K. Auernhammer[2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Leibniz Institute for Polymer Research, Dresden, Germany

Magnetorheological elastomers are hybrid materials comprising a non-magnetic polymer matrix with interspersed magnetic filler particles. As they are complementary to MR fluids and MR foams they gained a lot of interest for applications. To be useful the volume ratio of particles has to be in the order where the particle distance is roughly around one particle diameter. To get a basic idea of the mutual interaction under a rotating magnetic field we reduced the system to two superparamagnetic nickel particles enclosed by a PDMS-matrix. For the correct parameters of particle diameter, distance and elastic modulus of the surrounding matrix the system exhibit a new state described in the following: After applying the magnetic field particles snap into contact. During rotation the particles separate at certain points to take their original position. Thus the particle distance shows a hysteresis in relation to the angle between magnetic field and particle axes. Calculating the dipole interaction shows an agreement with the experiments even though in contact a treatment of the particles as point-like dipoles should be not valid. Presented state of the MREs needs to be compared to theoretical models.

CPP 59.4 Thu 16:00 H8

Simulation of magnetodielectric effect in magnetorheological elastomers — •Danil Isaev[1], Anna Semisalova[1,2], Yulia Alekhina[1], Liudmila Loginova[1,3], and Nikolai Perov[1,3] — [1]Lomonosov MSU, Faculty of Physics, Moscow, Russia — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Baltic Federal University, Kaliningrad, Russia

We present the computer model of the magnetodielecric effect (MDE) in magnetorheological elastomers. The effect is based on the assumption about the displacement of magnetic particles inside the elastic matrix under the external magnetic field and the formation of chain-like structures. Such displacement of metallic particles inside the elastic matrix of the sample between the planes of capacitor leads to the change of capacity, which can be considered as a change of effective dielectric permittivity of elastomer caused by magnetic field (MDE). In the model of the MDE the systems consist of around 100000 particles which are considered as isotropic and anisotropic samples varying with concentration of magnetic filler, size and space distribution of particles, elastic properties of the matrix. The influence of orientation of magnetic field and the capacitor plane was studied, the anisotropy of the effect was observed. The developed model resulted in a good qualitative agreement with experimental data obtained for Fe-based elastomers. It can be used to study these novel functional materials, analyze the features of magnetodielectric effect and predict the optimal composition of magnetorheological elastomers for further profound experimental study.

CPP 59.5 Thu 16:15 H8

Surface Lattice Resonances in the Visible Optical Range by Soft Lithography Templates and Directed Self-Assembly — •Vaibhav Gupta[1] and Töbias König[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e. V., hohe straße 6, D-01069 Dresden, Germany — [2]Cluster of Excellence Centre for Advancing Electronics Dresden, Technische Universität Dresden, Mommsenstraße 4, D-01062 Dresden, Germany

We demonstrate a novel approach towards cost-efficient and low-loss plasmonic nanostructures, whose pronounced optical anisotropy can be detected by naked eye. Soft interference lithography and template-assisted colloidal self-assembly are used to fabricate a flexible macroscopic periodic square lattice of gold nanoparticles. Surface scanning methods reveal a full coverage of the array. The high structural quality results in a narrow bandwidth surface lattice resonance with a line width of 25. We show the hybrid nature of the optical response using angle dependent UV-vis spectroscopy and numerical simulations. We propose a platform to curb the rigid nature of optical systems and offers versatile plasmon mode engineering. This real time band edge tunable metasurface can find potential application in long range coherent energy transfer. However the rational design framework established here allows for generalization in account for other wavelength regime and particle type.

15 min. break

CPP 59.6 Thu 16:45 H8

Disentangling the mechanical properties of polymer grafted nanoparticles — •Jiarul Midya and Arash Nikoubashman — Institute for Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany

Polymer grafted nanoparticles are promising materials with a wide range of applications in drug delivery, gas transport, photonic and electric materials. The mechanical properties of such materials can be controlled through the volume fraction and distribution of the nanoparticles, which can be achieved by changing the degree of polymerization of the grafted chains and their grafting density. Previous studies have tried to explain the elastic properties of nanocomposite materials through the effective medium theory, which relates the elastic modulus directly to the volume fractions of the hard nanoparticles and of the soft polymer matrix. However, recent experiments have shown significant variations of the elastic modulus for nanocomposites with the same volume fractions but different grafting densities and chain lengths. This behavior can not be explained by the existing effective medium theory. To investigate the origin of this effect we have performed molecular dynamics (MD) simulations. We demonstrate that the chain conformations play a crucial role for the elastic modulus of the nanocomposite, a contribution which has not been taken into account in the effective medium theory.

CPP 59.7 Thu 17:00 H8

Rigid Amorphous Phase in Polymer Nanocomposites as Revealed by Dielectric Spectroscopy and Fast Scanning Calorimetry — •Paulina Szymoniak and Andreas Schönhals — Bundesanstalt für Materialforschung und prüfung (BAM), Berlin, Germany

For inorganic/polymer nanocomposites a so-called Rigid Amorphous Phase (RAF) is formed in the interfacial region by adsorption of polymer segments onto the nanoparticles. The segmental dynamics of RAF is expected to be altered, as compared to the pure matrix, which might percolate to the entire system, affecting the overall nanocomposite properties. A combination of two relaxation spectroscopy techniques (Broadband Dielectric Spectroscopy (BDS) and Temperature Modulated DSC (TMDSC)) as well as Fast Scanning Calorimetry (FSC) were employed to investigate the structure and molecular mobility of nanocomposites based on Epoxy and Layered Doubled Hydroxides with different nanoparticle content. First, BDS investigations proved the existence of a process, which is present only for nanocomposites, assigned to the dynamics of polymer segments within RAF. Second, the amount of RAF was quantified by analyzing the change of specific heat capacity step of nanocomposites, comparing to the pure material. Thirdly, the glass transition of nanocomposites was studied with FSC, applying high heating rates (0.5-10 kK/s). Considering that all techniques probe essentially the same molecular process, an activation plot was constructed, delivering a complete picture of the molecular mobility and structure of the polymer nanocomposites including RAF.

CPP 59.8 Thu 17:15 H8

Implicit-medium model for viscoelastic properties of fractal-like aggregates polymer nanocomposites — •François Detcheverry[1], Yang Wang[1], Gaëtan Maurel[2], Marc Couty[2], and Samy Merabia[1] — [1]Univ Lyon, CNRS, Institut Lumière Matière, Villeurbanne, France — [2]MFP MICHELIN 23, Place des Carmes-Déchaux Clermont-Ferrand, France

Dispersing solid fillers into a polymer matrix is a common strategy to enhance its properties. Polymer nanocomposites (PNCs) so obtained with fractal-like aggregates have exceptional rheological behavior long exploited in the tire industry. However, due to disparity of time and length scales, our understanding of the relation between nanocomposites structure and rheology remains incomplete. Here, we propose a mesoscopic model to simulate fractal-like aggregate PNCs. While aggregates are represented explicitly, we use for the polymer matrix an implicit description based on generalized Langevin and Stokes equations, that capture the average effect of a viscoelastic medium. Such a two-level description allows us to simulate large PNCs systems containing dozens of aggregates. Investigating the linear viscoelastic properties of PNCs, we find that compared to nanoparticles, aggregates may induce levels of reinforcement considerably larger and we characterize the influence of aggregate size, rigidity and volume fraction. We also examine the Payne effect and relate it to the alignment of aggregates under the imposed deformation. Our results may help in building connections between the macroscopic mechanical response of the PNCs and the mesoscopic morphology of the fillers.

CPP 60: Biomaterials and biopolymers II (joint session BP/CPP)

Time: Thursday 15:00–17:00 Location: H10

CPP 60.1 Thu 15:00 H10

Cell Adhesion as a Function of Hydrogel Layer Thickness: From Thin Layers to Bulk Samples — •Sandra Sindt, Galen Ream, and Christine Selhuber-Unkel — Institute of Materials Science, CAU Kiel, Germany

Cells are in vivo in contact with a large range of different mechanical environments. However, many tissues have complicated structures without distinct elasticity values, which can result in stiffness gradients close to their interfaces and cells are known to be capable of sensing a more rigid substrate underneath a soft structure. For example, Buxboim et al. have recently shown that mesenchymal stem cells show increased adhesive spreading on thin soft hydrogels due to a stiff underlying substrate. A threshold of rigidity sensing of fibroblasts was reported to be 60-70 micrometer thickness at approximately 1 kPa of elastic modulus. We here report results on the dependency of cell adhesion on hydrogel thickness and elasticity. This is of great importance for the design and development of coatings for various biomedical applications. We use polyacrylamide layers on glass slides with thicknesses below 100 micrometer to semi-infinite bulk samples (ca. 500 micrometer). Furthermore, we use two different elasticities to determine, if the effective cellular substrate sensing depth is affected by the elasticity of the samples. Our results demonstrate that the spreading area and circularity is strongly influenced by the thickness of the polyacrylamide samples. However, there was no conclusive difference in this effect for both stiffnesses.

CPP 60.2 Thu 15:15 H10

Liquid-like protein condensates are glassy — •Louise Jawerth[1,2], Elisabeth Fischer-Friedrich[3], Suropriya Saha[1], Anthony Hyman[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Biotechnology Center, Technische Universitat Dresden

Liquid-like protein condensates (LLPCs) are intracellular compartments that segregate material without the use of a membrane. The liquid-like behavior of the condensates is a defining characteristic and the viscosity, surface tension and other material properties determine how segregated species diffuse into and within condensates; they, thus, critically impact the biological function of the condensates. It has become increasingly clear that some LLPCs do not have time-independent material properties, but can, instead, transition to more solid, gel-like materials. Here, we present our efforts to quantify these new materials as they age in vitro. We measure the visco-elastic material properties of two proteins, PGL-3 and FUS, by means of a combination of active and passive microrheology. At early times, we find that the droplets behave much like simple liquids but gradually become more elastic. Surprisingly, the changing mechanical properties can all be scaled onto a single master curve using one characteristic time scale which grows as the sample ages. This and other features we observe bear a striking resemblance to the behaviors observed in materials with glass-like aging suggesting that LLPCs are in fact not simple liquids but, rather, a type of soft glass.

CPP 60.3 Thu 15:30 H10

The Poisson ratio of the cellular actin cortex is frequency-dependent — Marcel Mokbel[1], Kamran Hosseini[2], Sebastian Aland[1], and •Elisabeth Fischer-Friedrich[2] — [1]Hochschule für Technik und Wirtschaft, Dresden, Germany — [2]Biotechnology Center, Technische Universität Dresden, Dresden, Germany

Cell shape changes are vital for many physiological processes such as cell proliferation, cell migration and morphogenesis. They emerge from an orchestrated interplay of cellular force generation and cellular force response both crucially influenced by the actin cytoskeleton. To model cellular force response and deformation, cell mechanical models commonly describe the actin cytoskeleton as a contractile isotropic incompressible material. However, in particular at slow frequencies, there is no compelling reason to assume incompressibility as the water content of the cytoskeleton may change. Here we challenge the assumption of incompressibility by comparing computer simulations of an isotropic actin cortex with tunable Poisson ratio to measured cellular force response. Comparing simulation results and experimental data, we determine the Poisson ratio of the cortex in a frequency-dependent manner. Our results show that the Poisson ratio of the cortex depends on the frequency and may deviate from the incompressible case. In addition, our results suggest that the assumption of cortex isotropy is violated at large time scales likely due to anisotropic actin cortex repolymerization from the membrane.

Invited Talk CPP 60.4 Thu 15:45 H10

3D scaffolds as cell-instructive biomaterials — •Christine Selhuber-Unkel — Institute for Materials Science, University of Kiel, Kiel, Germany

In vivo, many cell types are embedded in densely structured 3D environments. Such environments typically contain nano- and micropores or consist of nano- and microfibrous interwoven biopolymer structures. Mimicking such natural environments by synthetic materials can provide novel functionalities in many applications, particularly in tissue engineering. We therefore investigate 3D scaffold materials for their impact on cellular properties. As a first example, microchannels are embedded in a hydrogel matrix of well-defined stiffness, chemistry and conductivity. The scaffold provides a large and spatially controlled cell-surface contact area through the specific architecture of its pores, such that the specific properties of the environment have large impact on the cells and induce, e.g., cell capture. As a second example, carbon-based fibrous scaffolds will be introduced. These are highly attractive for applications that require conductive materials. In addition, they resemble the structural features of the natural extracellular environment and can be equipped with bioactive particles. Hence, 3D microstructured environments are promising candidates for instructing cells to execute specific and coordinated functions.

CPP 60.5 Thu 16:15 H10

Effect of drug treatment on the formation of malaria pigment crystals — •Szilvia Mucza[1], Ana Strinic[2], Agnes Orban[1], Petra Molnar[3], Peter Furjes[4], Beata Vertessy G.[3], and Istvan Kezsmarki[1,2] — [1]Department of Physics, Budapest University of Technology and Economics — [2]Experimental Physics V, University of Augsburg — [3]Hungarian Academy of Sciences Research Centre for Natural Sciences — [4]Institute of Technical Physics and Materials Science, Centre for Energy Research, Hungarian Academy of Sciences

The malaria pigment crystals are a by-product of the metabolic process of malaria parasites. These few-hundred-nanometer sized needle-like crystals are unique indicators of the presence of infection. Our group developed a magneto-optical device for malaria diagnosis, which can precisely measure the concentration of the crystals produced by the parasites. The increasing crystal concentration in time indicates the growth of the parasites in a culture, thus, the device is also sufficient for drug screening using parasite cultures. In the present study, we found that the magneto-optical method is able to determine the size distribution of the crystals in addition to their concentration. By following the size distribution of the crystals throughout the life cycle of the parasites for drug-treated and untreated cultures we could specify the stage when the drug action takes place. The same method can also be used to reveal if the drug action is related to the blocking of crystal formation or has a different pathway.

CPP 60.6 Thu 16:30 H10

Efficient hemozoin extraction from Plasmodium falciparum parasites — •Ana Strinic[1], Agnes Orban[2], Szilvia Mucza[2], Petra Molnar[3], Beáta Vértessy[3], Stephan Krohns[1], and Istvan Kezsmarki[1,2] — [1]Experimental Physics V, University of Augsburg — [2]Department of Physics, Budapest University of Technology and Economics — [3]Hungarian Academy of Sciences Research Centre for Natural Sciences

Hemozoin crystals are a natural biomarker of malaria infection. A prototypical magneto-optical setup uses magnetic and optical properties of hemozoin for a rapid and cheap, yet sensitive detection of malaria parasites within blood samples. As the parasites mature the volume of the crystallites produced within their food vacuole continuously increases. However, the age distribution of parasites within human blood and cell cultures is not homogenous. Thus, unveiling the relation between their age distribution and the size distribution of the hemozoin crystals may facilitate the monitoring of stage-specific drug actions and target oriented drug testing. Taking advantage of the high sensitivity of the magneto-optical method not only to the crystal concentration but also to their size distribution, we aim to determine the relation of size versus age distribution. This however strongly depends on a successful hemozoin extraction from in vitro cultures. Here, I show, how the crystal extraction process and sample preparation affect the quality of the extracted crystals and the magnitude of the magneto-optical signal. This allows determining the optimal procedure and investigating reactions along the preparation, which reduce the hemozoin concentration.

CPP 60.7 Thu 16:45 H10

Results of field trials of the rotating-crystal magneto-optical method for malaria detection — •Agnes Orban[1], Leandra Arndt[2], Tamarah Koleala[2], Jetsumon Sattabongkot[3], Stephan Karl[2], and Istvan Kezsmarki[1,4] — [1]Dept. of Phys., Budapest Uni of Tech. and Econ., Hungary — [2]Papua New Guinea Inst. of Med. Res., Madang, PNG — [3]Mahidol Vivax Res. Unit, Fac. of Tropical Medicine, Mahidol Uni, Bangkok, Thailand — [4]Exp. Phys. V, Center for Electronic Correlations and Magnetism, Uni. of Augsburg

Although malaria is still a global health burden, the current standard for its detection still remains the microscopic observation of stained blood smears. A novel cost-effective, automated, yet sensitive diagnostic method is needed for malaria detection both as an in-field instrument and as a laboratory tool.

Our group aims to design such a compact and inexpensive diagnostic device based on the detection of the magnetically induced linear dichroism exhibited by malaria pigment (aka. hemozoin). These micrometer-size crystals are promising malaria-diagnostic targets as they are unique indicators of the infection.

The rotating magnetic field employed in our system enables a very high sensitivity detection of hemozoin as tested on suspensions of synthetic crystals; on *Plasmodium falciparum* cultures, on mouse models and on human samples from field trials performed in Thailand and Papua New Guinea, the latter being the main focus of the talk.

CPP 61: Perovskite and Hybrid Photovolatics II (joint session HL/CPP)

Time: Thursday 15:00–17:30 Location: H36

CPP 61.1 Thu 15:00 H36

Valence band structure of CsPbBr$_3$ inorganic perovskite — •Janek Rieger[1], Daniel Niesner[1], Andrii Kanak[2], Petro Fochuk[2], Ievgen Levchuk[3], Christoph Brabec[3], and Thomas Fauster[1] — [1]Lehrstuhl für Festkörperphysik, University of Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]Department of General Chemistry and Material Science, Yuriy Fedkovych Chernivtsi National University, Kotsjubynskyi St. 2, Chernivtsi, 58012, Ukraine — [3]I-MEET, Department of Materials Science and Engineering, University of Erlangen-Nürnberg, Martensstr. 7, D-91058 Erlangen, Germany

The impact of the organic ion on the electronic properties of lead halide perovskites is matter of an ongoing debate. With angle-resolved photoelectron spectroscopy we investigated the properties of the valence bands of different perovskite single crystals cleaved in ultra-high vacuum. The talk focusses on recent results from the inorganic perovskite CsPbBr$_3$. Measurements were carried out in the temperature range from 87 K to 350 K, covering all bulk phase transitions of the material. The width of the valence band and the dispersion of the valence band maximum are discussed. Results are compared to the valence band structure of the organic-inorganic perovskite (HC(NH$_2$)$_2$)PbBr$_3$ as well as to (CH$_3$NH$_3$)PbBr$_3$, which was already investigated in detail by our group [1].

[1] D. Niesner et al., Phys. Rev. Lett. **117**, 126401 (2016).

CPP 61.2 Thu 15:15 H36

Charge Recombination Dynamics in Defect-Engineered Hybrid Organic-Inorganic Halide Perovskites — •Wen-Yu Cheng, Chang-Ming Jiang, and Ian Sharp — Walter Schottky Institut and Physik Department, Technische Universität München, 85748 Garching, Germany

Organic-inorganic halide perovskites, with their ease of fabrication and bandgap-tunability, provide promising prospects in photovoltaic and light-emitting diode applications. While such materials are highly tolerant of defects, the presence of ionic, along with electronic, charge conduction can result in dynamic optoelectronic properties. In this work, we aim at understanding the charge recombination pathways in defect-engineered perovskites. Point defects are intentionally and controllably introduced into the lattice of methylammonium lead iodide (MAPbI3), and a series of thin films with tunable bandgaps from 1.60 to 1.95 eV are fabricated. The concentrations and energetic positions of defects are quantified by photothermal deflection spectroscopy. The effects of these defects on photoluminescence yield are studied by steady-state and time-resolved fluorescence techniques. In addition to shedding light on the interactions between organics cations and the inorganic lattice, the results provide insights into the factors that underlie defect tolerance in hybrid halide perovskite semiconductors.

CPP 61.3 Thu 15:30 H36

Reversible Bandgap Instabilities in Multiple-Cation Mixed-Halide Perovskite Solar Cells — •Fabian Ruf[1], Pascal Rietz[1], Meltem F. Aygüler[2], Pablo Docampo[3], Heinz Kalt[1], and Michael Hetterich[1,4] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Department of Chemistry and CeNS, University of Munich (LMU), 81377 München, Germany — [3]Physics Department, School of Electrical and Electronic Engineering, Newcastle University, Newcastle upon Tyne, NE1 7RU, United Kingdom — [4]Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Multiple-cation mixed-halide perovskites have demonstrated their great potential as promising candidates for next-generation thin-film photovoltaics due to further improved power-conversion efficiency and stability. In this contribution, we investigate the stability of the compositional and resulting electronic structure of Cs$_{0.05}$(FA$_{0.83}$ MA$_{0.17}$)$_{0.95}$Pb(I$_{0.83}$Br$_{0.17}$)$_3$ solar cell absorbers using electroreflectance (ER) spectroscopy as sensitive and non-invasive measurement technique. Despite the enhanced compositional stability, these compounds show a decrease of the bandgap up to 70 meV under AM1.5 illumination and applied voltage. We attribute this to segregation of the intermixed perovskite into iodide-rich and bromide-rich domains which is also confirmed by in-situ X-ray diffraction. A detailed study under operation-relevant conditions (illumination and bias) is conducted in various environments (different oxygen contents and relative humidity) to evaluate the consequences for photovoltaic applications.

CPP 61.4 Thu 15:45 H36

Exciton Spin Dynamics and Their Dependence on Monovalent Cation Dipole Moment in Layered 2D Metal-Halide Perovskites — •Sean Bourelle, Ravichandran Shivanna, and Felix Deschler — University of Cambridge

Strong spin-orbit coupling in metal-halide perovskites connects optical transitions to spin states via the conservation of total angular momentum. These self-assembled quantum well structures of high-performance, defect tolerant semiconductors are broadly tunable through chemical composition. Here, we use ultrafast circularly-polarised broadband transient absorption spectroscopy to study the effect of perovskite composition on the polarisation and dynamics of exciton spin-states in two-dimensional (2D) Ruddlesden-Popper perovskites. We spectrally resolve the dynamic circular dichroism from a photoinduced polarisation in the secondary total angular momentum quantum number. This dichroism is used to determine the impact of the monovalent cation's dipole moment on the exciton spin-state depolarisation time.

CPP 61.5 Thu 16:00 H36

Vacuum-deposited Bismuth and 2D perovskites as absorber material for solar cells — •Martin Kroll — TU Dresden, IAPP, Dresden Deutschland

Organic-inorganic halide perovskites are a fast developing absorber material class for thin-film solar cells. The state of the art material combinations with record efficiencies all contain methyl-ammonium (MA) and lead as cations, which both display unfavorable properties. Cells with methyl-ammonium as organic cation all show rapid degradation due to its instability under exposure to light and moisture. Lead is known for its toxicity, which is bound to cause problems during cell marketing and legislation. In order to circumvent these issues, current research discusses less toxic material combinations like MA/Cesium-Bismuth-Iodide as well as self-layering 2D perovskites for better stability, which are formed by introducing large organic cations like butyl-ammonium (BA). So far, these approaches have only been shown using solution processing. We show the prospects of multi-source vacuum evaporation, which excels at material purity and film control. For MA/Cs3Bi2I9 as well as BA/MAPbI3, we present XRD and absorption data for thin-films as well as functional solar cells with efficiencies of > 1% and > 10%, respectively.

15 min. break

CPP 61.6 Thu 16:30 H36

The missing long range order in point-dipole based hybrid perovskite models — •Menno Bokdam and Jonathan Lahnsteiner — University of Vienna, Faculty of Physics and Center for Computational Materials Sciences, Vienna, Austria

The crystal structure of hybrid perovskites forms an intricate electrostatic puzzle. Using density functional theory (DFT) calculations we study the ordering of A={MA, Cs} cations in the APbI$_3$ perovskite framework. We show that previously proposed model Hamiltonians do not capture the long range structural order observed in large scale *ab-intio* molecular dynamics calculations. We attempt to improve on these models by applying an Ewald summation to sum the dipole-dipole interaction and by introducing a distance dependent screening function, however with only limited success. We envision that well-trained force fields would be able, and are likely necessary, to fully describe the finite temperature behaviour of hybrid perovskites.

CPP 61.7 Thu 16:45 H36

Recent progress in the vapour deposition of organic-inorganic hybrid metal-halide perovskite solar cells — •Juliane Borchert[1], Ievgen Levchuk[2], Lavina C. Snoek[1], Mathias Uller Rothmann[1], Henry J. Snaith[1], Laura M. Herz[1], Christoph J. Brabec[2], and Michael B. Johnston[1] — [1]Clarendon Laboratory, Department of Physics, University of Oxford — [2]Materials for Electronics and Energy Technology (i-MEET), FAU Erlangen-

Nürnberg, Erlangen, Germany

Hybrid metal-halide perovskite semiconductors are promising absorber materials for single junction and as well as for tandem solar cells. They have attracted a lot of research attention in recent years, due to the rapid rise of solar cell efficiencies for these materials. Record efficiencies have now reached to above 23%. Co-evaporation of perovskite thin-films for solar cells offers many advantages such as precise thickness control, pinhole free planar films and compatibility with a large range of different substrates. Efficient co-evaporated solar cells have been demonstrated with different perovskite materials, for example methylammonium lead iodide ($MAPbI_3$) and formamidinium lead iodide ($FAPbI_3$). Furthermore co-evaporation is a promising technique for the upscaling of perovskite solar cells to commercial scales. Some challenges remain, including problems with the process control and relatively small crystallites in the deposited films. Additionally, it is more challenging to achieve mixed compositions with co-evaporation than with solution processing. Here we present recent progress made towards solving these challenges.

CPP 61.8 Thu 17:00 H36

Growth Monitoring and Evolution of Optoelectronic Properties during the Formation of CH3NH3PbI3-xClx — •Klara Suchan[1], Justus Just[1], Eva L. Unger[1,2], José Marquez Prieto[2], and Thomas Unold[2] — [1]Lund University, Paradisgatan 2, 22350 Lund, Sweden. — [2]Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

We present a detailed investigation of the formation mechanism and the evolution of optoelectronic properties during annealing of chlorine derived methylammonium lead iodide (MAPIC). MAPIC layers are prepared by a one-step solution based process. While solution based processes do not need cost intensive vacuum technology and no high-temperature annealing steps, little is known about the exact mechanisms during synthesis. This prohibits identification and exact control of all relevant variables, leading to widely reported poor reproducibility. Using in-situ optical reflection we are able to monitor the evolution of the MAPIC phase as a function of time and processing temperature. The extracted formation kinetics are fitted using an altered Johnson-Mehl-Avrami-Kolmogorov model and show that the presence of Chlorine induces a delayed formation of MAPIC. This is verified by X-ray diffraction and X-ray fluorescence measurements. From absolute photoluminescence measurements we determine the quasi-Fermi level splitting during film formation. Correlating structural and electronic properties, we will present a detailed view on the reaction route during synthesis and specifically the influence of annealing conditions on the process and its intermediate states

CPP 61.9 Thu 17:15 H36

The versatility of polyelemental perovskite compositions — •Michael Saliba — University of Fribourg, Switerland

Perovskite solar cells (PSCs) have created much excitement in the past years and attract spotlight attention from research groups all over the world with many thousands of publications every year. This talk will provide an overview on the reasons for this unique success story highlighting the historic development as well as the specific material properties that make perovskites so attractive for the research community.

The current challenges are exemplified using a high-performance model systems for PSCs (multication Rb, Cs, methylammonium (MA), formamidinium (FA) perovskites).(1,2) The triple cation (Cs, MA, FA) achieves power conversion efficiencies (PCEs) close to 21% due to suppressed phase impurities. This results in more robust materials enabling breakthrough reproducibility. Through multication engineering, the seemingly too small Rb can be integrated (unsuited as a single-cation perovskite).(2) This results in a stabilized efficiency of 21.6%with one of the smallest differences between band gap and voltage ever measured for any PV material. Polymer-coated cells maintained 95% of their initial performance at elevated temperature for 500 hours under working conditions, a crucial step towards industrialisation of PSCs. The last part elaborates on a roadmap on how to extend the multicatio to multicomponent engineering providing a series of new compounds that are highly relevant candidates for the coming years.

CPP 62: Electrical, Dielectrical and Optical Properties of Thin Films

Time: Thursday 17:45–18:30 Location: H8

CPP 62.1 Thu 17:45 H8

Functional polymer thin films with tailored properties enabled by initiated chemical vapor deposition — Stefan Schröder, Frowin Ellermann, Maximilian Burk, Stefan Rehders, Cenk Aktas, Thomas Strunskus, and •Franz Faupel — Lehrstuhl für Materialverbunde, Technische Fakultät der Christian-Albrechts-Universität zu Kiel, Kaiserstr. 2, 24143 Kiel

Initiated chemical vapor deposition (iCVD) is a solvent-free, cost efficient technique to synthesize highly conformal organic thin films from the vapor phase. The polymer film properties can be precisely tuned by the deposition parameters, which enables the synthesis of tailored thin films in the ultrathin nanometer-range, as well as micrometer-range. This enables a wide field of applications for iCVD thin films like surface functionalisation, functional dielectrics and devices. We demonstrate conformal teflon coatings of complex 3d geometries, preparation of superior electret layers for application as sensors or for energy harvesting. Further we demonstrate adhesion promotion and incorporation of azo functionalities by use of different monomers within one iCVD process.

CPP 62.2 Thu 18:00 H8

Wrinkle Motifs: Gateways toward Flexible Optical Devices — •Anik Kumar Ghosh[1], Bernhard Alexander Glatz[1], Swagato Sarkar[1], Sven Wiessner[1], 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 Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, Germany

Wrinkled patterns are the result of mechanical 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 enabling them for enhanced light-matter interactions. Furthermore, the aforementioned wrinkling technique provides an alternative route towards large area fabrication of grating-waveguide resonant structures. These by the virtue of flexibility can find application in opto-mechanics as well as deformed based resonance sensors following guided mode resonance (GMR).

CPP 62.3 Thu 18:15 H8

Exciton binding energy of organic materials: ground-state vs. excited-state charge-transfer complexes — •Andreas Opitz[1], Paul Beyer[1], Norbert Koch[1,2], and Wolfgang Brütting[3] — [1]Humboldt-Universität zu Berlin — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — [3]Universität zu Berlin Augsburg

Organic semiconductors are materials with a high exciton binding energy (EBE), which significantly affects their electronic and optical properties. The EBE is the difference between the electronic gap (obtained by direct and inverse photoelectron spectroscopy) and the lowest optical transition energy (determined from absorption spectroscopy). In this contribution, the EBE is investigated for thin films of pristine organic semiconductor as well as charge-transfer complexes.

The EBE of pristine diindenoperylene (DIP) is about 0.50 eV. DIP combined with fullerene as acceptor was studied for photovoltaic cells and the very weak absorbtion exhibits an EBE of approx. 0.07 eV. A comparably low value was determined for the weakly interacting ground-state CTC of DIP with a dicyanoperylene-bis(dicarboxyimide) derivative (PDIR-CN2). The acceptor hexafluorotetracyano-naphthoquinodimethane (F6TCNNQ) forms a strongly interacting ground-state CTC with DIP and reveals an EBE of 0.79 eV.

The CTCs have to be distinguished by ground-state (GS) and excited-state (ES) interaction, which we will relate to the determined EBEs. The properties of the CTC excitons range here from CT to Frenkel like and are strongly dependent on interaction scheme between donor and acceptor.

CPP 63: Annual General Meeting of the CPP Division (CPP Mitgliederversammlung)

Time: Thursday 18:45–19:45 Location: H13

Duration 60 min.

CPP 64: Active Matter III (joint session BP/CPP/DY)

Time: Friday 9:30–12:00 Location: H11

CPP 64.1 Fri 9:30 H11

Dynamics of an active model microswimmer in an anisotropic fluid — •Abdallah Daddi-Moussa-Ider and Andreas M Menzel — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Düsseldorf

Several recent experiments investigate the orientational behavior of self-propelled bacteria and colloidal particles in anisotropic fluids such as nematic liquid crystals. Correspondingly, we study theoretically the dynamics of a simple model microswimmer in a uniaxially anisotropic fluid. The behavior of both puller- and pusher-type swimmers in the anisotropic fluid is analyzed. Depending on the propulsion mechanism as well as the relative magnitude of different involved viscosities, we find alignment of the microswimmer parallel or perpendicular to the anisotropy axis. The observed swimmer reorientation results from the hydrodynamic coupling between the self-induced fluid flow and the anisotropy of the host fluid. Our theoretical predictions are found to be in qualitative agreement with recent experiments on swimming bacteria in nematic liquid crystals. They support the objective of utilizing the anisotropy of a surrounding fluid to guide individual swimmers and self-propelled active particles along a requested path, enabling controlled active transport.

Reference: A. Daddi-Moussa-Ider and A. M. Menzel. Dynamics of a simple model microswimmer in an anisotropic fluid: Implications for alignment behavior and active transport in a nematic liquid crystal, Phys. Rev. Fluids 3, 094102 (2018).

CPP 64.2 Fri 9:45 H11

Dynamics of bottom-heavy squirmers — •Felix Ruehle and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Germany

The self-propulsion of biological or synthetic microswimmers is often influenced by a gravitational field [1,2], where a density mismatch leads to sedimentation and an offset center of mass triggers reorientation along the direction of gravity so that they swim upwards [2]. Combining these passive effects with the non-equilibrium properties of active motion creates novel and interesting dynamics, both in dense and dilute suspensions [3]. In particular, a large variety of dynamical behaviours has been observed for the squirmer microswimmer model [4,5].

In this contribution we focus on bottom-heavy squirmers and determine their state diagram, depending on the gravitational force and acting torque. For strong gravitational forces we observe conventional sedimentation, whereas the density profile is inverted for weaker forces. Additionally, we find stable convective plumes for neutral squirmers that become metastable as the torque increases. We also observe spawning clusters at the bottom if the sedimentation velocity almost equalizes the swimming speed. Spawning clusters and continuous plumes do not occur for pusher and puller type swimmers.

[1] J. Palacci, et al., *Phys. Rev. Lett.* **105**, 088304 (2010).
[2] K. Drescher et al., *Phys. Rev. Lett.* **102**, 168101 (2009).
[3] K. Wolff, A. M. Hahn and H. Stark, *EPJE* **36**, 1 (2013).
[4] J.-T. Kuhr et al., *Soft Matter* **13**, 7548 (2017).
[5] F. Rühle et al., *New J. Phys.* **20**, 025003 (2018).

CPP 64.3 Fri 10:00 H11

Bead-spring modelling of triangular microswimmers — •Sebastian Ziegler[1], Alexander Sukhov[2], Jens Harting[2,3], and Ana-Sunčana Smith[1,4] — [1]PULS Group, Institute for Theoretical Physics, Department of Physics, Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Germany — [3]Dep. of Applied Physics, Eindhoven University of Technology, The Netherlands — [4]Division of Physical Chemistry, Ruder Bošković Institute Zagreb, Croatia

A customary approach to model mechanical micropropulsion is to prescribe the swimming stroke. However, with this approach, the hydrodynamic features of the motion are in essence smoothed over and the problem becomes a purely geometrical one. The alternative approach, yet significantly more demanding, is to impose not the stroke itself but the forces driving the device. The swimming stroke then emerges as a result of the various forces acting in the system. We use a perturbative approach to examine a triangular swimmer's behaviour in the Stokes regime that is also eligible for general geometries of bead-spring swimmers. The device shows a multifaceted comportment dependent on a number of therefore identified effective parameters. The triangular swimmer is further used as a prototype to study the influence of variations in the viscosity of the surrounding fluid on its motion.

CPP 64.4 Fri 10:15 H11

Simple Swimmers Reverse Direction near a Surface — •Michael Kuron[1], Philipp Stärk[1], Joost de Graaf[2], and Christian Holm[1] — [1]Institut für Computerphysik, Universität Stuttgart, Deutschland — [2]Institute for Theoretical Physics, Universiteit Utrecht, Nederland

The motion of a microswimmer can change substantially in the presence of a surface. Sperm are known to move in circular trajectories near a wall, paramecia move in sinusoidal trajectories through a tube, and chemical swimmers can orbit around spherical obstacles. Spherical squirmers are one of the simplest model microswimmers, commonly defined by the first two Legendre modes of their surface slip velocity. In this talk, we use the squirmer to numerically investigate the effect of the environmental geometry. We discuss how the transition between scattering and orbiting/hovering depends on the strength of the squirmer's hydrodynamic dipole moment. Interestingly, we observe cases where the squirmer orbits/hovers along a surface in a direction opposite to that observed in bulk. This effect is present both in a far-field theoretical model and our lattice Boltzmann calculations, which accurately account for the near-field flow. These results extend the understanding of the effect of geometry on microswimmer motion and show the importance of finite swimmer size and associated near-field effects.

CPP 64.5 Fri 10:30 H11

Bacterial Swarming Dynamics — •Hannah Jeckel[1,2,3], Eric Jelli[1,2], Raimo Hartmann[1], Praveen Singh[1], Rachel Mok[3,4], Jan Frederik Totz[5], Lucia Vidakovic[1], Bruno Eckhardt[2], Jörn Dunkel[3], and Knut Drescher[1,2] — [1]Max Planck Institute for Terrestrial Microbiology, Marburg, Germany — [2]Department of Physics, Philipps-University Marburg, Germany — [3]Department of Mathematics, Massachusetts Institute of Technology, Cambridge, MA — [4]Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA — [5]Institute for Theoretical Physics, Technical University Berlin, Germany

Coordinated dynamics of individual components in active matter are an essential aspect of life on all scales. Establishing a comprehensive, causal connection between intracellular, intercellular, and macroscopic behaviors has remained a major challenge due to limitations in data acquisition and analysis techniques suitable for multiscale dynamics. Here, we combine a high-throughput adaptive microscopy approach with machine learning, to identify key biological and physical mechanisms that determine distinct microscopic and macroscopic collective behavior phases which develop as *Bacillus subtilis* swarms expand over five orders of magnitude in space. Our experiments, continuum modeling, and particle-based simulations reveal that macroscopic swarm expansion is primarily driven by cellular growth kinetics, whereas the microscopic swarming motility phases are dominated by physical cell-cell interactions. These results provide a unified understanding of bacterial multi-scale behavioral complexity in swarms.

CPP 64.6 Fri 10:45 H11

Effects of collective bacterial motility on their chemotactic navigation — •Remy Colin and Victor Sourjik — Max Planck

Institute for Terrestrial Microbiology, Marburg, Germany

At high cell density, swimming bacteria exhibit collective motility patterns, self-organized through physical interactions of a however still debated nature. Although high-density behaviors are frequent in natural situations, it remains unknown how collective motion affects chemotaxis, the main physiological function of motility that enables bacteria to follow chemical and other gradients in their environment. Here, we systematically investigated this question in the model organism *Escherichia coli*, varying cell density, cell length and suspension confinement. The characteristics of the collective motion indicated that its emergence is dominated by hydrodynamic interactions between swimmers. We observed that moderate increase in cell density enhanced the chemotactic drift of bacteria, whereas it was suppressed at higher densities, because the collective motion disturbed the choreography necessary for chemotactic sensing. We suggest that this physical hindrance imposes a fundamental constraint on high-density behaviors of motile bacteria, including swarming as well as the formation of multicellular aggregates and biofilms.

CPP 64.7 Fri 11:00 H11

Feedback Control of Active Microswimmers — •Alexander Fischer[1], Haw Yang[2], and Frank Cichos[1] — [1]Uni Leipzig — [2]Princeton University

Collective motion created by the interaction of autonomous individuals plays a major role in flocks of birds, bacterial growth or the motion of robotic swarms. Sensing and reacting to signals is a fundamental issue of life. Microswimmers, which are artificial objects that mimic the active motion of biological systems, do not have such sensing and response features built in yet, but may gain them through an external control of their propulsion. Here we explore an information exchange between artificial microswimmers by computer-controlled feedback processes. We have created a setup where multiple active microswimmers can react to their position in space or their distance to other microswimmers. We investigate the influence of different interaction potentials or a delay in the information exchange. Our results demonstrate so far that particles can be coupled to each other by the used feedback by designed virtual potentials. The collective motion of such coupled particles reveals oscillating modes with emergent features like spontaneous rotation. The experiments shall help to understand the emergence of complex behavior in biological systems.

CPP 64.8 Fri 11:15 H11

Out-of-plane beating components of active axonemes isolated from Chlamydomonas reinhardtii — Azam Gholami[1], •Soheil Mojiri[2], Eberhard Bodenschatz[1], and Jörg Enderlein[2] — [1]Max-Planck Instiute for Dynamics and Self-Organization, Göttingen, Germany — [2]Georg-August Universität, Göttingen, Germany

Cilia and flagella are ubiquitous in the living world. They are essential for micro-scale driven transport of fluids or cells by cilia/flagellar beating. Their slender bodies are composed of a microtubule/molecular motor structure that when taken independently are called an axoneme. Axonemes move by bending waves that emerge from the interplay between internal stresses generated by dynein motor proteins . Here we use the novel multi-plane phase contrast imaging technique to record the three dimensional beating pattern of isolated axonemes from Chlamydomonas reinhardtii that beat in the vicinity of a substrate. We measure the torsion of the axoneme along the contour length with high spatiotemporal resolution. High precision information on out-of-plane beating component of axonemes allows us to check the validity of the resistive-force theory.

CPP 64.9 Fri 11:30 H11

Nanoscale chemotaxis of enzymes and small molecules — •Jaime Agudo-Canalejo[1,2], Tunrayo Adeleke-Larodo[1], Pierre Illien[3], and Ramin Golestanian[4,1] — [1]University of Oxford, Oxford, UK — [2]Penn State University, State College, USA — [3]ESPCI Paris, Paris, France — [4]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

We present a microscopic theory for the observed chemotaxis of enzymes and other small molecules. [1,2] We find that two distinct mechanisms contribute to enzyme chemotaxis: a diffusiophoretic mechanism due to non-specific interactions, and a new type of mechanism due to binding-induced changes in the diffusion coefficient of the enzyme. For a typical enzyme, the two mechanisms compete against each other, one dominating at high substrate concentration, the other at low concentration. The competition between the two mechanisms may be used to engineer nanovehicles that move towards or away from regions with a specific substrate concentration. Finally, we include the effects of anisotropy and flexibility of the enzyme, [3] and show that enzymes can be aligned by gradients, and shape fluctuations lead to corrections in the diffusion and chemotactic mobility of enzymes. [1] Agudo-Canalejo, J., Adeleke-Larodo, T., Illien, P., & Golestanian, R. (2018) Acc. Chem. Res. 51, 2365 [2] Agudo-Canalejo, J., Illien, P., & Golestanian, R. (2018) Nano Lett. 18, 2711 [3] Adeleke-Larodo, Agudo-Canalejo, J., & Golestanian, R. (2018) arXiv:1811.09631

CPP 64.10 Fri 11:45 H11

High-motility visible light-driven Ag/AgCl Janus microswimmers interacting with passive beads — •xu wang[1], larysa baraban[2], vyacheslav r misko[3,4], franco nori[4,5], petre formanek[6], tao huang[2], gianaurelio cuniberti[2], jürgen fassbender[1], and denys makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorfe.V., Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]Universiteit Antwerpen, B-2610 Antwerpen, Belgium — [4]RIKEN Cluster for Pioneering Research, 351-0198 Saitama, Japan — [5]University of Michigan, 48109-1040 Michigan, USA — [6]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany

Visible light driven nano/micro swimmers typically show mean squared displacement (MSD) values in the range of up to 200 μm^2 (over 10 s) under favorable UV light illumination.[1] Here, we demonstrate Ag/AgCl-based spherical Janus micromotors that reveal an efficient propulsion with a MSD to 3000 μm^2 (over 10 s) in pure H_2O under visible blue light illumination (λ = 450-490 nm).[2] Furthermore, we show the micromotors reveal efficient exclusion effect to their surrounding passive polystyrene beads in pure H_2O experimentally and using numerical simulations of the Langevin equations.[3]

1. Simmchen, J., et al., ChemNanoMat 2017, 3, 65.
2. Wang, X., et al., Small DOI: 10.1002/smll.201803613.
3. Wang, X., et al., Small 2018, 14, 1802537 (Frontispiece paper)

CPP 65: Two-dimensional Materials IV (joint session HL/CPP)

Time: Friday 9:30–13:00 Location: H36

CPP 65.1 Fri 9:30 H36

Optical Valleytronic Properties of CVD-grown Tungsten Disulfide AA' and AB Bilayers — •Lorenz Maximilian Schneider[1], Jan Kuhnert[1], Simon Schmitt[1], Ulrich Huttner[1], Lars Meckbach[1], Tineke Strouken[1], Stepan W. Koch[1], Wolfram Heimbrodt[1], Shichen Fu[2], Xiaotian Wang[2], Kyung Nam Kang[2], and Arash Rahimi-Iman[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, D-35032 Marburg, Germany — [2]Department of Mechanical Engineering, Stevens Institute of Technology, Hoboken, New Jersey, 07030, USA

Two-dimensional semiconductors such as transition-metal dichalcogenides have attracted considerable attention due to their strong light-matter interaction as well as "valleytronic" properties. The valley-dependent polarization properties are of potential interest for future devices and, both, homojunctions as well as heterostructures of monolayer materials promise considerable valley-polarization degrees and valley coherence.

In this work, chemical-vapour-deposition-grown AA' and AB stacked tungsten-disulfide bilayers are investigated. The differences between AA' and AB stacked bilayers are characterized optically and attributed to the distinct interlayer coupling between k-space valleys. Our spectroscopic investigations are supported by calculations focusing on the difference in symmetry and interlayer electronic coupling for these bilayers. A comparably high valley polarization and valley coherence is found for the AB stacked case in contrast to the AA' case, which is in good agreement with the expectations.

CPP 65.2 Fri 9:45 H36

Exciton-lattice coupling in monolayer WSe2 investigated by femtosecond electron diffraction — •Shuo Dong[1], Daniela Zahn[1], Robert Schneider[2], Thomas Vasileiadis[1], Helene Seiler[1], Yingpeng Qi[1], Rudolf Bratschitsch[2], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Institute of Physics and Center for Nanotechnology, University of Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

Exciton-phonon coupling as the essential exciton relaxation mechanism plays a crucial role in transition metal dichalcogenides (TMDC). Besides the bright exciton dynamics, the formation of dark excitons greatly impacts the optoelectronic properties of atomically thin TMDC, which requires spin flip-scattering or phonon-assisted momentum transfer. Here, we investigate the incoherent lattice excitation associated with exciton relaxation in monolayer WSe2 by femtosecond electron diffraction. We discuss the observed structural dynamics in terms of the intra- and inter-valley exciton scattering towards the lower-lying dark states. The direct measurement of lattice motion provides important complementary insights to exciton dynamics.

CPP 65.3 Fri 10:00 H36

Towards an Atomistic Understanding of Defects in 2D Materials - Correlating Defects, Band Structure and Excitons — •Christoph Kastl[1], Roland Koch[1], Chris Chen[1], Bruno Schuler[1], Johanna Eichhorn[1], Soren Ulstrup[2], Aaron Bostwick[1], Chris Jozwiak[1], Nicholas Borys[3], Francesca Toma[1], Shaul Aloni[1], Alexander Weber-Bargioni[1], Eli Rotenberg[1], and Adam Schwartzberg[1] — [1]Lawrence Berkeley National Laboratory, Berkeley, United States — [2]Aarhus University, Denmark — [3]Montana State University, Bozeman, United States

Despite their importance, a detailed understanding of defects in 2D materials and their impact on excitonic and electronic properties is lacking. We use spatially resolved, angle resolved photoemission spectroscopy (nano-ARPES) to map the variations in band structure and defect density of monolayer WS_2 down to a resolution of 150 nm. [1] By correlating nano-ARPES with photoluminescence, we reveal the interplay between local defect density, band structure, and excitons. We compare this to atomic force and scanning tunneling microscopy, where we unambiguously identify defects at the atomic level. Surprisingly, the chalcogen vacancy is not present in as-grown monolayers, although it is commonly inferred to be the dominant point defect.[2] Instead, we find that substitutional oxygen effectively passivates chalcogen vacancies, which removes the electronic in-gap state and renders correct assignment of the defect challenging.

[1] C. Kastl et al., 2D Mater. 5, 045010, 2018. [2] arXiv:1810.02896, arXiv:1810.03364.

CPP 65.4 Fri 10:15 H36

Magnetic Anisotropic Behavior in Two-Dimensional Layered $Cr_2Ge_2Te_6$ Crystals — •Sebastian Selter[1,2], Gaël Bastien[1], Anja U. B. Wolter[1], Saicharan Aswartham[1], and Bernd Büchner[1,2] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany

$Cr_2Ge_2Te_6$ is one of the few known examples of two-dimensional layered ferromagnetic insulators. Ferromagnetic order was observed down to the bilayer, while theoretical calculations even suggest stable ferromagnetic order on the monolayer. This finding makes this compound interesting in terms of both fundamental understanding as well as for novel spintronic applications.

Thus, to entangle the physics behind possible monolayer ferromagnetism it is essential to understand the bulk magnetism which will enable us for the future applications. Here, we present a comprehensive synthesis, magnetic and thermodynamic investigation on $Cr_2Ge_2Te_6$. Bulk $Cr_2Ge_2Te_6$ becomes ferromagnetic below 64 K with the magnetic easy axis parallel to the crystallographic *c*-axis. A magnetic anomaly has been observed for low external fields applied perpendicular to the easy axis. An investigation of the field dependency of this anomaly hints towards a field driven nature.

CPP 65.5 Fri 10:30 H36

Nanoscale Mapping of Charge Transfer at SnS/MoS_2 2D-2D p-n Junctions Created via Low-Temperature Epitaxy — •Alex Henning[1,2], Jack N. Olding[1,3], Michael J. Moody[1], Jason Dong[1], Emily A. Weiss[3], and Lincoln J. Lauhon[1] — [1]Department of Materials Science and Engineering, Northwestern University, USA — [2]Walter Schottky Institute and Physics Department, Technische Universität München — [3]Department of Chemistry, Northwestern University, USA

Many novel two-dimensional (2D) van der Waals (vdW) heterostructures with intriguing properties for optical and electronic applications have been created by mechanical exfoliation and stacking. The ability to directly grow vdW heterostructures over large areas would create new opportunities for large-scale integration. Here, p-type tin sulfide (SnS) is grown on n-type molybdenum disulfide (MoS_2) in an atomic layer deposition (ALD) reactor at low temperatures (180 °C) to form vertical p-n 2D-2D heterojunctions (HJs). X-ray diffraction and electron backscatter diffraction establish an axiotaxial relationship between the two crystals. Kelvin probe force microscopy (KPFM) combined with a tunable illumination source is used to characterize the topography, potential landscape and photoresponse of the MoS_2/SnS HJs with a lateral resolution < 50 nm. The gained structural and electronic properties were used to optimize the parameters for the growth of electronically active SnS of controlled thickness. The built-in potential difference of 0.9 eV, measured between MoS_2 and SnS, is significantly larger than those previously reported for 2D HJs.

CPP 65.6 Fri 10:45 H36

Controlling band alignment at heterointerfaces using atomically thin Janus structures with built-in dipoles — •Simone Manti — Technical University of Denmark, Kongens Lyngby, Denmark

Recently Janus MoSSe monolayers have been synthesized by replacing S by Se on one side of MoS2. This material is an example of an atomically thin Janus structure, in which the inversion symmetry in the plane is broken leading to a finite out of plane dipole moment. Here we demonstrate that by inserting a MoSSe layer between two semiconductors, or between a semiconductor and a metal, it is possible to control the band alignment, or Schottky barrier, at the interface in a highly predictable manner. Using high-throughput density functional theory (DFT) calculations we screen for new, stable 2D Janus structures. This leads to a library of potentially synthesizable 2D materials with out-of-plane dipoles of varying strength corresponding to potential shifts between 0 and 2 eV. Our work opens new directions for rational design of band alignment at heterointerfaces.

15 min. break

CPP 65.7 Fri 11:15 H36

Theory of electron-exciton scattering in atomically thin semiconductors — Christian Fey[1], Peter Schmelcher[1], Atac Imamoglu[2], and •Richard Schmidt[3] — [1]Universität Hamburg, Germany — [2]ETH Zürich, Switzerland — [3]MPI of Quantum Optics, Garching, Germany

Excitons interacting with charge carriers in van-der-Waals materials represent a new venue to study the many-body physics of strongly interacting Bose-Fermi mixtures. In order to derive an effective low-energy model for such systems we develop an exact diagonalization approach that predicts the bound and scattering properties of electron, excitons, and trions in two-dimensional semiconductors. By solving the quantum mechanical three-body problem of interacting charge carriers we obtain binding energies of excitons and trions that are in excellent agreement with quantum Monte Carlo predictions. Importantly, in our approach also excited states are accessible. This allows us to study exotic excited trion states as well as to predict the scattering phase shifts of electrons and excitons. From these results we derive an effective low-energy model of exciton-electron scattering that can serve as an input to advanced many-body techniques. As a demonstration we study the recently observed exciton Fermi polarons, and we show that effective range corrections predicted by our model have a substantial impact on the optical absorption spectrum of charge-doped transition-metal dichalcogenides. Our approach can be applied to a plethora of many-body phenomena realizable in atomically thin semiconductors ranging from exciton lattices and localization to induced superconductivity.

CPP 65.8 Fri 11:30 H36

Computational characterization of novel 2d-materials for applications in energy and electronics — •Davide Campi[1], Thibault Sohier[1], Cedric Klinkert[2], Simran Kumari[1], Marco Gibertini[1], Nicolas Mounet[1], Mathieu Luisier[2], and Nicola Marzari[1] — [1]École polytechnique fédérale de Lausanne, Lausanne, Switzerland — [2]ETH Zurich, Zurich, Switzerland

Novel materials are crucial to future progress in information-and-communications technologies (ICT) and in energy harvesting, conversion, and storage. 2D materials provide an entire novel playground to discover novel properties and functionalities. The recent identification of many novel monolayers [1] has made available a large portfolio of materials to be explored. In this work we present an applications-oriented screenings aimed at the identification of the most promising candidates for photocatalytic water splitting, field-effect transistor channels and superconductivity.

CPP 65.9 Fri 11:45 H36

Magnetic hallmarks of viscous electron flow in graphene — •Karina A. Guerrero-Becerra[1], Francesco M. D. Pellegrino[2,3], and Marco Polini[1,4] — [1]Istituto Italiano di Tecnologia, Via Morego 30, 16163 Genova, Italy — [2]Dipartimento di Fisica e Astronomia, Università di Catania, Via S. Sofia, 64, I-95123 Catania, Italy — [3]INFN, Sez. Catania, I-95123 Catania, Italy — [4]School of Physics & Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom

Electrical transport, thermal transport, and scanning gate spectroscopy measurements have been used to identify signatures of viscous electron flow in graphene, PdCoO2, and GaAs. In this regime of transport, viscosity determines electron whirlpools in the steady-state current pattern. So far, a direct experimental observation of electron whirlpools and associated backflow is still lacking. We predict that the profile of the magnetic field generated by hydrodynamic electron flow in confined geometries displays unambiguous features linked to whirlpools and backflow near current injectors. We also show that the same profiles shed light on the nature of the boundary conditions describing friction exerted on the electron fluid by the edges of the sample. Our predictions are within reach of vector magnetometry based on nitrogen-vacancy centers in diamond, a technique that access the details of 2D spatial flow patterns in graphene [1] and combines the benefits of high spatial resolution, competitive magnetic field resolution, and operability over a wide range of temperatures.

[1] J.-P. Tetienne et. al., Sci. Adv. **3**, e1602429 (2017).

CPP 65.10 Fri 12:00 H36

Strain-induced localization of interlayer excitons in a van-der-Waals heterostructure — Malte Kremser, •Moritz Meyer, Janine Gückelhorn, Kai Müller, and Jonathan Finley — Walter Schottky Institut, Technische Universität München, München, Deutschland

The intricate potential landscape of interlayer excitons (IX) in heterobilayers (HBLs) of transition metal dichalcogenides is currently undergoing intense study. [1, 2] We show that strain can be utilized to locally modify the IX potential resulting in locally trapped states, similar to the strain-related emergence of quantum emitters in monolayer WSe2. [3, 4]

We locally strain a HBL composed of MoSe2 and WSe2 by placing it on top of lithographically defined nanopillars. The strain at the nanopillar positions creates localized states that appear as new peaks in low-temperature photoluminescence (PL) measurements, red-shifted by ~50-100 meV with respect to the IX main emission. We show that in excitation-power-dependent measurements the emission features a series of discrete peaks that suggests sequential charging of the trapping potential with multiple IXs.

[1] K. Tran et al., arXiv 1807.03771

[2] K. L. Seyler et al., arXiv 1809.04562

[3] A. Branny et al., Nat. Commun. 8, 15053 (2017)

[4] C. Palacios-Berraquero et al., Nat. Commun. 8, 15093 (2017)

CPP 65.11 Fri 12:15 H36

Extreme Ultraviolet Core-Exciton Dynamics in Two-dimensional Molybdenum Disulfide — •Michael Zürch[1,8], Hung-Tzu Chang[1], Alexander Guggenmos[1], Diana Y. Qiu[2,3], Romain Geneaux[1], Yen-Chang Chen[4,5], Xuan Wei[5], Chang-Ming Jiang[6,7], Yufeng Liang[4], Felipe H da Jornada[2,3], Adam Schwartzberg[4], David Prendergast[4], Vincent C. Tung[5], Steven G. Louie[2,3], Daniel M. Neumark[1,6], and Stephen R. Leone[1,2,6] — [1]Department of Chemistry, University of California, Berkeley, USA — [2]Department of Physics, University of California, Berkeley, USA — [3]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, USA — [4]Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, USA — [5]School of Engineering, University of California, Merced, USA — [6]Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, USA — [7]Joint Center of Artificial Photosynthesis, LBNL, Berkeley, USA — [8]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Novel tightly-bound core-excitons triggered by an XUV attosecond pulse are observed in two-dimensional transition-metal dichalcogenide molybdenum disulfide. State-of-the-art theory calculations confirm the observed features. The dynamics observed in the core-exciton states between the molybdenum 4p and 4d states indicate coherences, and population transfer between different states. The observation of strongly enhanced long-lived core excitons in two-dimensional semiconductors paves the way for further exploration into the properties of core excitons in two-dimensional materials and potential application of these.

CPP 65.12 Fri 12:30 H36

One-Nanometer-Thin Carbon Nanomembranes: Combining High Water Permeance with High Selectivity — •Yang Yang, Petr Dementyev, Niklas Biere, Daniel Emmrich, Patrick Stohmann, Riko Korzetz, Xianghui Zhang, André Beyer, Sascha Koch, Dario Anselmetti, and Armin Gölzhäuser — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

Membrane-based separation provides an energy-efficient technology in producing clean water. Recent nanotechnology breakthroughs have led to the emergence of 2D membranes which promise minimal transport resistance and thus exceedingly high molecular flow rates. Carbon nanomembranes (CNMs) are a special class of 2D materials made by crosslinking of self-assembled monolayers. In this work, we will present the rapid and selective water permeation through a 1.2-nm thin CNM fabricated from terphenylthiol (TPT) precursors [1]. TPT CNMs consist of sub-nanometer channels with a high areal density of $10^{18}\,\mathrm{m}^{-2}$. The membrane can block the passage of most gases and liquids, while permitting water and helium to pass through. In particular, water transits with a remarkably high permeance of 1.1×10^{-4} mol $\mathrm{m}^{-2}\,\mathrm{s}^{-1}\,\mathrm{Pa}^{-1}$, 2,500 times faster than helium. The rapid water flow is ascribed to a hydrogen-bonded cooperative transport inside the CNM channels.

Reference

[1] Y. Yang, *et al.* Rapid Water Permeation Through Carbon Nanomembranes with Sub-Nanometer Channels. *ACS Nano* 2018, 12, 4695-4701.

CPP 65.13 Fri 12:45 H36

Photoactive molecular nanosheets with 1 nm thickness — •Maria Küllmer[1], Felix Herrmann-Westendorf[1,3], Stefan Götz[2], Christof Neumann[1], Patrick Endres[2], Andreas Winter[2], Ulrich Sigmar Schubert[2,4], Benjamin Dietzek[1,3,4], and Andrey Turchanin[1,4] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Institute of Organic Chemistry and Makromolecular Chemistry (IOMC), Friedrich Schiller University Jena, 07743 Jena — [3]Leibniz Institute of Photonic Technology e. V., 07745 Jena — [4]Center for Energy and Environmental Chemistry Jena (CEEC Jena), 07743 Jena

Artificial photocatalytic systems play an important role in the development of novel energy sources. Functional incorporation of molecular catalysts into two-dimensional (2D) soft matter matrixes is a prerequisite towards the realization of the artificial leaf systems. Here we present 1 nm thick photoactive molecular nanosheets - Carbon Nanomembranes (CNMs) - generated by electron irradiation induced crosslinking of self-assembled photocatalytic ruthenium-(II)-complexes on gold substrates. We characterize the chemical and structural properties of these molecular 2D systems using high-resolution X-ray photoelectron and surface enhanced Raman spectroscopy in combination with atomic force and scanning electron microscopy. We employ photothermal deflection spectroscopy to characterize the adsorption band of the formed free-standing photoactive CNMs and to compare it with the characteristics of the pristine ruthenium-(II)-complexes

CPP 66: Organic Electronics and Photovoltaics V - Semiconducting Properties and Devices

Time: Friday 9:45–12:00 Location: H18

Invited Talk CPP 66.1 Fri 9:45 H18

Coupled Organic-Inorganic Nanostructures for Optical Switches — •Marcus Scheele — Universität Tübingen, Tübingen, Deutschland

Optical switches are key components for data processing on the basis of silicon photonics, in which they perform the crucial conversion of a photonic information from an optical fiber into an electric information for a silicon-based processing unit. The status of the switch is controlled by an external light source, emitting at a wavelength suitable to be absorbed by the conductive channel to photo-induce additional charge carriers and modulate the current output of the switch in close analogy to a classic transistor. This presentation details how hybrid superlattices of semiconducting nanocrystals and organic pi-systems with long-range order are applied as active layers in functional optical switches. The particular novelty for optical switching is an activated absorption mechanism, in which stimulation with one optical signal sensitizes the material towards an amplified recognition of a second optical stimulus. Several examples with different material combinations are presented and the importance of exciton formation as well as charge transfer across the inorganic-organic interface is discussed.

CPP 66.2 Fri 10:15 H18

Comparative Study of Semiconductivity in 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. Often they exhibit large pores, into which small molecules may be absorbed. While many potential applications for semiconductive MOFs in e. g. sensors or electrocatalysis are imaginable, only very few examples of non-insulating MOFs have been found to date. Theoretical studies indeed suggest, that pure MOF bulk crystals have insufficient intrinsic charge carrier density to show finite conductivity. It is generally suggested that this drawback is overcome by defects in the crystal structure for the few known conductive MOFs. However, the intrinsic carrier density is only one factor governing electrical conductivity, with the other major contribution being the charge carrier's mobility. This, we study in bulk MOF crystals using a band transport model and thereby establish an upper limit estimate for the mobility. We outline the factors limiting the mobility exemplarily for $M(ta)_2$ MOFs where M stands for different transition metal centers. These share the same crystal structures but vary strongly in their carrier mobilities, hinting at first design criteria for future semiconducting MOFs.

CPP 66.3 Fri 10:30 H18

Electrostatically designed metal-organic frameworks based p-i-n junctions — •Giulia Nascimbeni[1], Christof Wöll[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Institute of Functional Interfaces, Karlsruhe Institute of Technology, Germany

Metal-organic frameworks (MOFs) are highly crystalline porous materials consisting of metal ions or clusters coordinated mostly by oxygen or nitrogen atoms and connected by organic linkers. The nearly unrestricted choice of linkers and metal nodes leads to a variety of different materials, whose properties can be tuned simply by changing their chemistry. Recently new possible applications of MOFs in electronics and photonics [1, 2] have been suggested based on engineering their electronic band structures [3, 4]. In the spirit of this band structure engineering, in this contribution we present an innovative approach based on the layer-by-layer assembly of surface-anchored MOFs (SURMOFs) [5], which allows to integrate electric fields into molecular thin films, thus mimicking the electronic structure of p-i-n junction present in solar cells. We use band structure calculations to show how this can be achieved via the controlled manipulation of the potential energy landscape in MOFs through the regular assembly of dipolar molecules. [1] Sun et al., Angew. Chem. Int. Ed., 2016, 55, 3566. [2] Neumann et al., ACS Nano, 2016, 10 (7), 7085. [3] Pham et al., J. Phys. Chem. C, 2014, 118, 4567. [4] Park et al., J. Am. Chem. Soc., 2015, 137, 1774. [5] Liu et al., Chem. Soc. Rev., 2017, 46, 5730.

CPP 66.4 Fri 10:45 H18

High-Speed and High-Current Vertical Organic Transistors — •Felix Dollinger[1], Henning Iseke[1], Kyung-Geun Lim[2], Axel Fischer[1], Petr Formánek[3], Hans Kleemann[1], and Karl Leo[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Dresden, Germany — [2]Korea Research Institution for Standard Science (KRISS), Daejeon, Korea — [3]Leibniz-Institut für Polymerforschung Dresden e. V. (IPF), Dresden, Germany

Organic thin-film transistors enable light-weight, inexpensive and flexible electronic applications. The Organic Permeable Base Transistor (OPBT) is a vertical transistor design that allows for very high current densities, and hence the fastest operating speed of all organic transistors with transit frequency reaching 40 MHz [Kheradmand-Boroujeni et al., 2018].

We will explain the operating mechanism for OPBTs and give insights into optimizations of the base oxide layers and investigations on the stability of the device.

The modulation of current in an OPBT is achieved by a metallic base electrode that is located in the center of the vertical stack. In the on-state, this thin aluminum electrode is permeable for electrons. It is passivated by a native oxide layer to prevent leakage current. We have been able to significantly improve the oxide layer and reduce parasitic leakage currents. Electrical stress measurements on OPBTs help to understand the suitability of these transistors for long-time real-life applications. Illustrative TEM images will be shown to clarify the device's structure and function.

15 min. break

CPP 66.5 Fri 11:15 H18

Determination of the Equilibrium Charge Distribution by Impedance Spectroscopy of P-Doped Organic Semiconductors — •Victoria Wissdorf[1,2], Markus F116ricks[2,3], Christof Pflumm[1], Wolfram Jaegermann[2,3], and Eric Mankel[2,3] — [1]Merck KGaA, Darmstadt — [2]Technische Universität Darmstadt, Darmstadt — [3]InnovationLab, Heidelberg

Impedance spectroscopy is a powerful tool to investigate the intrinsic properties of organic semiconductors. One possibility is, to link capacitance voltage measurements at zero bias voltage to the interface energy level alignment of doped hetero-junctions [1]. This description is based on the assumption that the capacitance is solely determined by the metal-semiconductor contact [1],[2]. With this Mott-Schottky approach any additional contributions from interfaces, injection barriers or space charge regions inside the device are neglected. Furthermore, the measured p-doping dependence cannot be explained within the framework of this picture. Within this work we present a theoretical description that couples a continuous equivalent circuit model with the solution of the drift-diffusion equation for equilibrium. This approach yields a direct link between the material parameters and interfaces to the results of impedance spectroscopy measurements. We furthermore compare the theoretical model to measurements of p-doped single layer devices and can explain how the material and device parameters change with varied p-doping concentration.

[1] Lee et al., Adv. Funct. Mater. 22, 855-860 (2012)

[2] R.L. Anderson, Solid-State Electronics 5, 341 (1962)

CPP 66.6 Fri 11:30 H18

Remote doping at organic heterointerface — •Ilia Lashkov, Kevin Krechan, Katrin Ortstein, Hans Kleemann, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials, Nöthnitzer Str. 61, 01187 Dresden, Germany

Organic and molecular electronics is a novel field of microelectronics that provides the possibility of producing electronic devices onto flexible substrates and at a low process temperature. However, organic thin-film transistors suffer from a low charge carrier mobility which lowers their potential for applications. Both problems have been successfully solved in inorganic electronics by the concept of remote doping. In our work, we investigate remote doping at a junction between two organic semiconductors with a different energy gap. The offset of valence states leads to charge carrier transfer from the wide gap semiconductor. Charge transfer at the interface between the organic semiconductors is investigated by in-situ conductivity measurements during film deposition. We directly monitor the charge transfer by means of the film conductivity which experiences a sudden increase upon the deposition of the first molecular monolayer of the narrow gap material onto the wide gap semiconductor. Additionally, we investigate the transfer by ultra-violet photo-electron spectroscopy (UPS) and present first steps towards the realization of a remotely doped organic thin-film transistor.

CPP 66.7 Fri 11:45 H18

Electronic interactions in precursor solution of F4TCNQ doped P3HT polymers — •Vandana Tiwari[1], Hong-Guang Duan[1,2,3], Ajay Jha[1], 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

Unraveling the favorable electronic interaction between dopant and polymer is the key to the success of molecular doping in organic semiconductors. Here we use two-dimensional electronic spectroscopy to explore the electronic dynamics of F4TCNQ-doped conducting polymer, P3HT in precursor solution mixtures. The electronic interactions among the ion-pairs formed in precursor solutions are captured in the form of off-diagonal peaks connecting the electronic states of polymer and dopant radicals. We have theoretically modeled our system to simulate the experimental data and achieve a quantitative picture of the Coulombic interaction between cation and anion radicals in solution. Our study reveals the heterogeneous electronic interactions that possibly serve as a seed for the structures in the spin-casted films.

CPP 67: Polymer and Molecular Dynamics, Friction and Rheology

Time: Friday 9:45–12:15 Location: H13

CPP 67.1 Fri 9:45 H13

Nanomechanische Charakterisierung von funktionalen Celluloseeinzelfasern — •Julia Auernhammer[1] und Robert Stark[2] — [1]Technische Universität Darmstadt, Insitut Materialwissenschaften, Physics of Surfaces, Alarich-Weiß-Straße 16, 64287 Darmstadt — [2]Technische Universität Darmstadt, Insitut Materialwissenschaften, Physics of Surfaces, Alarich-Weiß-Straße 16, 64287 Darmstadt

Der heutige Alltag ist ohne Applikation von Papier, wie in Printmedien, Verpackungsprodukte oder gar in technischen Spezialpapieren, kaum vorstellbar. All diese Anwendungen machen sich die einzigartigen Eigenschaften von Papier zu nutze. Papier ist porös und kann ohne externe Pumpen kapillargetrieben Flüssigkeiten transportieren. Im Vergleich zu porösen Kunststoffen ist es chemisch und thermisch stabiler, reißfest und kann nach Gebrauch rezykliert oder energetisch verwertet werden. Zum Design von Papieren mit funktionalen Eigenschaften werden die Papiere oft mit hydrophoben Polymeren modifiziert um die Nassreißfestigkeit zu verbessern. Mit Hilfe der Rasterkraftmikroskopie und der Korrelation zur Konfokalmikroskopie und Fluoreszenzmikroskopie wird hier ein detailreiches Bild der Verteilung des Polymerfilms auf einzelnen Cellulosefasern aufgezeigt. Zudem wird die räumliche Ausdehnung der Einzelfaser bei steigender Luftfeuchtigkeit sowie die damit verbundenen Veränderungen der lokalen mechanischen Eigenschaften an der Oberfläche der Einzelfaser herausgearbeitet. Weiterhin zeigt der Mikrozugversuch am Rasterkraftmikroskop das Verhalten von Einzelfasern bei mechanischer Beanspruchung unter verschiedenen Luftfeuchtigkeiten.

CPP 67.2 Fri 10:00 H13

Non-monotonic particle size effect on the glass transition in polymer-particle blends and its application to shape memory polymers — Elias M. Zirdehi and •Fathollah Varnik — ICAMS, Ruhr-Universität Bochum, Germany

The addition of small molecules is found to enhance the dynamics of structural relaxation in polymers and glasses [1]. This effect turns out to be a non-monotonic function of the particle size [2]. Through a detailed analysis of the non-Gaussian parameter for the particles and monomers, it is shown that the time scales of cooperative motion for the two constituents exhibit a separation when decreasing the size of particles. This decoupling of dynamics is also apparent in the ratio of diffusion coefficient and relaxation times of two species. Loss of the coupling effect makes the monomers become weakly influenced by the fast dynamics of the smaller particles. On the other hand, the larger particles are strongly coupled to polymers while being less mobile, which leads to a rather weak enhancement effect on the polymers dynamics. The strongest effect on polymers dynamics is observed in the intermediate particle sizes where the particles have high mobility as well as sufficiently strong coupling to the polymer matrix. A potential application of this effect can be the tuning of the triggering temperature in shape memory polymers. This issue is also briefly discussed.

1. Elias Mahmoudinezhad, Axel Marquardt, Gunther Eggeler and Fathollah Varnik, Procedia Computer Science 108, 265-271 (2017).
2. Elias M. Zirdehi, Fathollah Varnik, Non-monotonic particle size effect on the glass transition in polymer-particle blends (under rev.).

CPP 67.3 Fri 10:15 H13

Rheology of Nonequilibrium Polymer Melts — •Manjesh K. Singh, Hsiao-Ping Hsu, and Kurt Kremer — Max Planck Institute for Polymer Research, Mainz, Germany

Polymers have become very popular in everyday use because of ease in processing of polymeric materials. Polymers are processed to different complex shapes from the molten state. Polymer melts display rich viscoelastic behavior in the typical length and time scales. The processing of polymer melts become difficult with increase in molecular weight (Mw) because of increase in viscosity. The long polymer chains in a melt have to move in a specific way due to the topological constraints ”entanglements” imposed by neighboring chains. This happens because of the fact that the in a polymeric systems each monomers are connected to their neighboring monomers and can not crossover each other. Increase in number of entanglements with increase in Mw leads to increase in viscosity.

We have used complementary experimental and simulation approaches to study the development of entanglements in a fully disentangled melt of collapsed polymer chains and changes in viscosity, moduli and glass-transition temperature during the process.

CPP 67.4 Fri 10:30 H13

Cyclization and relaxation dynamics of finite-length collapsed self-avoiding polymers — •Julian Kappler[1,2], Frank Noé[1], and Roland R. Netz[1] — [1]Freie Universität Berlin, 14195 Berlin, Germany — [2]Cambridge University, Cambridge CB3 0WA, United Kingdom

The loop formation kinetics of polymers governs the dynamics of protein folding and gene expression regulation. The quantity of main interest is the cyclization time τ_{cyc}, i.e. the mean time it takes the two polymer ends to find each other. We study the cyclization and relaxation dynamics of ideal as well as interacting polymers as a function of chain length N. For the cyclization time of ideal chains we recover the known scaling $\tau_{\mathrm{cyc}} \sim N^2$, for a self-avoiding slightly collapsed chain we obtain from Langevin simulations and scaling theory a modified scaling $\tau_{\mathrm{cyc}} \sim N^{5/3}$. The cyclization and relaxation dynamics of a finite-length collapsed chain scale differently; this unexpected dynamic multi-scale behavior is rationalized by the crossover between swollen and collapsed chain behavior.

CPP 67.5 Fri 10:45 H13

Network dynamics in hydrogen-bonding telechelic polymers: associate lifetime, structural relaxation and phase separation — •Martin Tress[1], Kunyue Xing[1], Pengfei Cao[2], Shiwang Cheng[3], 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 — [3]Michigan State University, Department of Chemical Engineering and Material Science, East Lansing, Michigan, United States

Supra-molecular networks formed by reversible bonds between polymer chains exhibit extraordinary properties, e.g. extreme toughness & elongation at break or self-healing. We study short telechelic polymers with different H-bonding ends and backbones [Xing, Tress et al., Macromolecules 10.1021/acs.macromol.8b01210]. The H-bonds increase the glass transition temperature (Tg), though in flexible polydimethyl siloxanes it does not vary with H-bond strength whereas in much stiffer polypropylene glycol Tg varies significantly. In contrast, viscosity strongly depends on H-bond strength in the former while it is unchanged in the latter. Complementary measurements of mechanical and dielectric relaxation indicate that this due to competing lifetimes of supra-molecular associations and chain relaxation. Furthermore, viscoelastic properties are enhanced tremendously by phase separating ends, controlled by Tg of these aggregates. The concept of bond lifetime renormalization [Stukalin et al., Macromolecules 46 (2013) 7525] describes the results qualitatively but appears to fail quantitatively.

15 min. break

CPP 67.6 Fri 11:15 H13

Filtering polymeric topologies in spatially-modulated nano channels — •Lisa B. Weiss[1], Mattia Marenda[2], Cristian Micheletti[2], and Christos N. Likos[1] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria — [2]SISSA, International School of Advanced Studies, via Bonomea 265, I-34136 Trieste, Italy

Polymers of various topologies are of importance in biology, rheology and material science. Macromolecules of distinct topology consist of the same type and number of monomers, making it challenging to separate them using chemical approaches. Nevertheless, topology influences strongly their response to flow fields in concentrated and dilute solutions. Previously, successful separation strategies for linear and circular polymers have been developed, which unfortunately fail in the case of knotted ring polymers. Thus, we present a novel separation strategy employing spatially-modulated channels, building up on topology-dependent diffusivities in such channels. We take hydrodynamic interactions via the multi-particle collision algorithm into account. In equilibrium, we find an astonishing inversion of diffusivities in modulated channels compared to bulk, which can be rationalized by a Fick-Jacobs approach. Applying a flow enables a reliable separation of circular polymers from their knotted counter parts in weak flows. Looking in detail at the relevance of the size of the narrowing, we identify a regime of strong restrictions on polymer translocations in the case of pore sizes smaller than the average knot size. Here, the essential crossings act as a parachute preventing translocation.

CPP 67.7 Fri 11:30 H13

Accelerating molecular dynamics simulations with population annealing — •Henrik Christiansen[1], Martin Weigel[2], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany — [2]Applied Mathematics Research Centre, Coventry University, Coventry CV1 5FB, England

We adapt Population Annealing to Molecular Dynamics simulations and demonstrate its ability to accurately simulate systems with rugged-free energy landscapes. For this we simulate the folding of met-enkephalin, a short peptide commonly used to test the performance of algorithms. A comparison with Parallel Tempering, the de facto standard for the simulation of complex systems with a rugged free-energy landscape using Molecular Dynamics, is presented. Further, we show that it is possible to use adaptive temperature steps in Population Annealing, i.e., the temperature set has not to be known beforehand, like in Parallel Tempering, but can be determined on-the-fly.

CPP 67.8 Fri 11:45 H13

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 is 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 the self-assembly of diblock copolymers, as the synthesis of these macromolecules is well-established. 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 significantly alter their rheological properties due to entanglement effects. Thus, it is important to consider the chain conformations on a microscopic level to fully understand the macroscopic flow properties of the melts. The arrangement of the individual polymers, and hence 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. As a first step, we studied through self-consistent field theory (SCFT) the domain spacing and the loop and bridge distribution of lamella-forming multiblock copolymers in equilibrium, and found semiquantitative agreement with experiments. We then combined SCFT with molecular dynamics simulations of Lennard-Jones chains to determine the anisotropic shear viscosity of block copolymer melts.

CPP 67.9 Fri 12:00 H13

Influence of interface hydration on sliding of graphene and molybdenum disulfide single-layers — •Hu Lin, Abdul Rauf, Nikolai Severin, Igor M. Sokolov, and Jürgen P. Rabe — Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Humidity influences friction in layered materials in peculiar ways. For example, while water improves the lubricating properties of graphite, it deteriorates those of molybdenum disulfide (MoS2). The reasons remain debated, not the least due to the difficulty to experimentally compare dry and hydrated interface frictions. For this, we strain the mica substrate and detect strain in graphene and MoS2 by changes in Raman and photoluminescence spectra, respectively. The spectra show that the hydration of interfaces between a mica substrate and single-layers of graphene and MoS2 with a molecularly thin water layer affects strain transfer from the substrate to the 2D materials. Strain relaxation in graphene changes from stick-slip in dry contact, to viscous when hydrated. In contrast, there is no viscous relaxation in MoS2 regardless of hydration. Our work provides a novel approach for better understanding the impact of hydration on friction in layered materials.

CPP 68: Microfluidics (joint session DY/CPP)

Time: Friday 10:00–12:15 Location: H6

CPP 68.1 Fri 10:00 H6

Tunable stirring of the interior of biofluid microdroplets in a microfluidic channel — •Pierre-Yves Gires, Mithun Thampi, and Matthias Weiss — Experimental Physics I, University of Bayreuth, Germany

Studying dynamic changes of and within fluid droplets with biomimetic or biological composition, e.g. produced in microfluidic devices, is a key technique for biotechnology. However, due to their small dimensions, a controlled and gentle stirring of the droplets' interior has been very challenging. Here we report on an approach that allows for performing such a tunable stirring of microdroplets via home-made magnetic nano-stir bars. In particular, we have used a PDMS-based microfluidic junction with a hydrophobic carrier fluid to produce aqueous biofluid droplets with 10-100 microns diameter into which magnetic nano-stir bars were incorporated. By subsequent stimulation with an alternating magnetic field, nano-stir bars performed a rotational motion with tunable frequencies in the range 0.01-10 Hz. The differential effect of this stirring on particle diffusion and on the undulation of semiflexible biofilaments, i.e. microtubules, was then quantified via quantitative fluorescence microscopy to dissect thermal and active noise contributions.

CPP 68.2 Fri 10:15 H6

Soft particles in inertial microchannel flow — •Christian Schaaf and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

Particles immersed in an inertial microchannel flow at intermediate Reynolds numbers move towards discrete equilibrium positions in the channel cross section. This Segré-Silberberg effect can be explained by the inhomogeneous shear profile of Poiseuille flow and particle-wall interactions. While rigid particles assemble around halfway between channel walls and channel center, deformable capsules move closer towards the center [1]. In addition to this lateral inertial focusing, rigid particles at low densities also assemble on 1D lattices along the flow [2]. In this contribution we aim to understand how the deformability of elastic capsules influences the lattice formation and what novel structures now develop.

To study this problem we conduct lattice-Boltzmann simulations. As a first step we focus on the dynamics of a flowing particle pair and see how inertia changes the dynamics of a pair of deformable capsules. For a pair of rigid particles we have recently found that the dynamics is dominated by viscous forces at small distances and by inertial forces at larger distances [3].

In the end these results are used to explain the behavior of soft particle trains and to analyze their dynamics and stability.

CPP 68.3 Fri 10:30 H6

Focusing and splitting of particle streams in microflows via viscosity gradients — •Matthias Laumann and Walter Zimmermann — University of Bayreuth, Germany

Microflows are intensively used for investigating and controlling the dynamics of particles, including soft particles such as biological cells and capsules. A classic result is the tank-treading motion of elliptically deformed soft particles in linear shear flows, which do not migrate across straight stream lines in the bulk. However, soft particles migrate across straight streamlines in Poiseuille flows. In this talk we present a new mechanism of cross-streamline migration of soft particles. If the viscosity varies perpendicular to the stream lines then particles migrate across stream lines towards regions of a lower viscosity, even in linear shear flows. An interplay with the repulsive particle-boundary interaction causes then focusing of particles in linear shear flows with the attractor stream line closer to the wall in the low viscosity region. Viscosity variations perpendicular to the stream lines in Poiseuille flows leads either to a shift of the particle attractor or even to a splitting of particle attractors, which may give rise to interesting applications for particle separation. The location of attracting streamlines depend on the particle properties, like their size and elasticity. The cross-stream migration induced by viscosity variations is explained by analytical considerations, Stokesian dynamics simulations with a generalized Oseen tensor and Lattice-Boltzmann simulations.

CPP 68.4 Fri 10:45 H6

Synchronization between two boiling bubbles — •Claus-Dieter Ohl[1,2], Dang Minh Nguyen[1,2], Muttikulangara Swaminathan Sanathanan[3], Jianmin Miao[3], and David Fernandez Rivas[4] — [1]Otto-von-Guericke University, Institute for Physics, Magdeburg. — [2]School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore. — [3]School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapore. — [4]Mesoscale Chemical Systems, Faculty of Science and Technology, University of Twente, Enschede, The Netherlands

Acoustically driven bubbles are nonlinear oscillators showing a wide range of behaviours such as period-doubling bifurcations, deterministic chaos, and synchronization to an external signal. Here we demonstrate that bubbles driven with a constant heat source can couple with each other and yield in-phase synchronization, even in the absence of an external sound field. Besides perfect synchronization we resolve the parameter space where independent oscillations and bubble merging occurs. The main finding that only weakly oscillating bubbles synchronize provides a path for experimental scale-up to study spatio-temporal synchronization. In the wider scope the findings are relevant for heat transfer applications from structured heaters where complex multi-bubble oscillations are expected.

CPP 68.5 Fri 11:00 H6

Dissipative particle dynamics simulation for viscosity behavior induced by self-assembly of surfactants confined in nanotubes — •Yusei Kobayashi and Noriyoshi Arai — Kindai University, Higashiosaka, Japan

Self-assembly is one of the most studied branches of materials chemistry, and has attracted a lot of attention due to its diverse potential applications in electronics, engineering, biomedical, and optical fields. Thus far, many previous studies have reported on the self-assembly of surfactants in solution for developing various functional materials. On the other hand, the chemical nature of the wall surface on the nano/micro scale is another key parameter which can drastically change the self-assembled structures. To study such wall-induced effects on the self-assembled structures and their rheological properties, we performed computer simulations of surfactant solutions in chemically distinct nanotubes under pipe flow. In particular, we determined the shear viscosity as a function of (local) shear rate in hydrophilic, hydroneutral, and hydrophobic nanotubes at different surfactant concentrations. Here, we found that the addition of surfactant molecules led to characteristic viscosity behaviors with rich steady-state morphologies.

15 min. break

CPP 68.6 Fri 11:30 H6

Particle trajectory entanglement in confined fluidic systems — •Alvaro Marin[1], Massimiliano Rossi[2], and Christian J. Kähler[2] — [1]Physics of Fluids, University of Twente, The Netherlands — [2]Bundeswehr University Munich, Germany

Suspensions in motion can show very complex and counterintuitive behavior, particularly at high concentrations. However, in this work we show how suspensions at substantially lower dilute concentrations can develop complex dynamics. Such non-trivial dynamics appear when particles tend to interlace their trajectories, only bonded by hydrodynamic interactions. Using a fairly simple system of non-Brownian particles flowing in a confined channel, we reveal a rich complexity in the particle dynamics due to the dominance of short-range particle-particle and particle-wall hydrodynamic interactions. Such rich dynamics are revealed and studied via experiments and particle dynamics simulations, resulting in a very good quantitative comparison.

CPP 68.7 Fri 11:45 H6

Aligning beads with boxing gloves — •Archit Bhatnagar[1], Anatol Fritsch[1], Matthäus Mittasch[1], Michael Nestler[2], Matthias Loidolt[1], Axel Voigt[2], and Moritz Kreysing[1] — [1]MPI of Cell Biology, Dresden — [2]Department of Mathematics, TU Dresden

Recently we have described that we can move the cytoplasm of cells and developing embryos in a non-invasive manner. For this we made use of thermoviscous flows (1).

Here we ask the question if these long-ranged flow fields can in principle also be used for the precision alignment of colloids, an endeavor that seems as reasonable as trying to align small beads while wearing boxing gloves. Simulations, however, suggest that series of flow fields can be found to align multiple colloids at the same time, even if these particles are closely spaced.

We follow this strategy experimentally and will report the feasibility, precision limits due to the brownian motion of particles, and prospects for colloidal physics and applications in biology.

References: (1) Mittasch et al., " Non-invasive perturbations of intracellular flow reveal physical principles of cell organization", Nature Cell Biology 1 (2018)

CPP 68.8 Fri 12:00 H6

Anisotropic thermophoresis and thermal orientation of elongated colloids — •Marisol Ripoll and Zihan Tan — Institute of Complex Systems, Forschungszentrum Jülich, Germany

Anisotropic phoresis refers to the different phoretic response that elongated particles can have as a function of their relative orientation with a gradient of temperature or concentration. These effects can further be enhanced when the surface of the system is not homogeneous, case in which an additional phoretic orientation can appear for non-fixed colloids [1]. Investigations are performed by a hydrodynamic mesoscale simulation approach [2]. The anisotropic phoresis can furthermore be applied to the design of phoretic micromachines and micropums, which shows to provide an alternative to the conventional application of external forcing in order to pump fluids at the microscale [3].

[1] Z. Tan, M. Yang, and M. Ripoll, Soft Matter 13, 7283 (2017) Z. Tan, PhD thesis, Universität zu Köln (2018)

[2] D. Lüsebrink, M. Yang, and M. Ripoll, J. Phys.: Condens. Matter 24, 284132 (2012) M. Yang, and M. Ripoll, Soft Matter 9, 4661 (2013)

[3] M. Yang, R. Liu, M. Ripoll, and K. Chen, Nanoscale 6, 13550 (2014); Lab Chip, 15, 3912 (2015)

CPP 69: Glasses and Glass transition (joint session DY/CPP)

Time: Friday 10:00–11:45 Location: H19

CPP 69.1 Fri 10:00 H19

Unified Formulation of Fractional Relaxation — •Tillmann Kleiner and Rudolf Hilfer — Institut für Computerphysik, Universität Stuttgart

Susceptibility functions that involve stretching exponents which are derived from fractional dynamics [1] reproduce the excess wing of α-relaxation peaks that has been observed in dielectric spectra of glass forming materials [2]. The contemporary formulation of fractional dynamics requires two distinct approaches to describe the relaxation motion and the response of the system to periodic excitations. The former uses fractional Liouville-Caputo derivatives in the time domain and the latter multiplication with the susceptibility function in the frequency domain. Both approaches impose severe restrictions on the past history of the involved electric field that are unrealistic in an experimental situation. Due to the occurrence of memory effects this poses a serious problem. In this contribution a unified description of fractional dynamics is presented where fractional derivatives are defined using distributional convolution. The resulting response functions are stretched multinomial Mittag-Leffler functions. This formulation extends the mentioned approaches to all experimentally relevant situations in a consistent way and exposes a high degree of convenience.

[1] R. Hilfer, Analysis **36**, 49-64 (2016)
[2] F. Kremer and A. Loidl, The Scaling of Relaxation Processes, Springer, (2018)

CPP 69.2 Fri 10:15 H19

Ion and Molecule Transport in Nanopores - a NMR Study — •Christoph Säckel, Sarah Schneider, and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstr. 6, 64289, 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 biological ion channels are highly selective and sensitive, they lack the robustness for technological applications. In contrast, silica pores are well-established in industrial environments, but possess inferior capabilities, e.g. no selectivity. A hybrid system would combine the favourable properties of both types of pores. It is therefore necessary to understand the influence of the confinement on the temperature-dependent ion and molecule transport. We systematically vary the pore parameters and study effects on the dynamics with ^{1}H, ^{2}H and ^{7}Li nuclear magnetic resonance (NMR). We combine homogeneous and gradient field NMR to selectively investigate water and ion dynamics on broad time and length scales in the supercooled regime. Both the local and long-range dynamics of ions and water show a slowdown with decreasing pore size. In addition, our data indicates more heterogeneous dynamics for the liquid in confinement than in bulk. Both the slowdown and heterogeneity can be explained by a slower layer of solution at the pore walls and bulk-like dynamics in the pore centre. Self-diffusion shows an Arrhenius-like behaviour of the solution in confinements, while bulk samples are best described by a VFT fit.

CPP 69.3 Fri 10:30 H19

Glass transition of water-like models in bulk and confinement — •Robin Horstmann and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstr. 6, 64289, Darmstadt, Germany

Tetrahedral network formers have a special position among glass-forming liquids. Their well defined local prefered structures cause significant structural changes with temperature but often render the transfer of models of supercooled liquids, e.g. density scaling, difficult. We use molecular dynamics simulations to examine two families of water-like molecules, based on the SPC/E and TIP4P/2005 water models, that vary only in their partial charges to systematically alter the strength of the hydrogen-bonds and, hence, the relevance of tetrahedral order.^{1} The varied inter-molecular interactions spread dynamics 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. Additionally, we study water-like systems in neutral confinements and find unchanged tetrahedral structure but slowed molecular dynamics. To describe the glassy slowdown, we assume that the activation free energy can be split into a constant value E_∞ and an exponentially growing contribution $E_c(T)$.^{2} Common ratios of E_∞/T_g and $E_c(T)/T_g$ are found indicating that the high temperature results can be used to rescale the glassy slowdown in bulk and confinement.

[1] R. Horstmann and M. Vogel, J. Chem. Phys. **147**, 034505 (2017)
[2] B. Schmidtke et al., Phys. Rev. E **86**, 041507 (2012)

CPP 69.4 Fri 10:45 H19

Effects of fractional freezing on the structure and dynamics of deeply cooled confined water — •Sebastian Kloth and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstr. 6, 64289, Darmstadt, Germany

The properties of confined water are of enormous importance in nature and technology. In particular, the effects of partial freezing on structure and dynamics is largely relevant for, e.g. geology, cryopreservation and our understanding of the glass transition of water [1]. To obtain a better understanding of the properties of the liquid fraction molecular dynamic simulations were performed with the TIP4P/Ice water model. This model was chosen for its good agreement with several water and ice properties. A series of frozen confinements with different pore diameters were made to analyze the structure and dynamics of the water layer remaining liquid upon deeply cooling, between pore wall and ice crystals. The partial freezing results in altered water dynamics, most importantly, the non-Arrhenius behavior of weakly supercooled bulk water is replaced by an Arrhenius behavior. Confined and bulk water have in common that the structure is disturbed at low temperatures. Either trough the existence of two interfaces in the case of the frozen confinement or through partly forming ice nuclei in the bulk.

[1] Cerveny, S. et al., Chem. Rev., **2016**, *116* (13)

CPP 69.5 Fri 11:00 H19

Decoding of the Toric Code: A High Temperature Series Analysis — •Benedikt Placke[1], Nikolas Breuckmann[2], and Ananda Roy[1,3] — [1]JARA Institute for Quantum Information, RWTH Aachen University — [2]Department of Physics and Astronomy, University College London — [3]Insitut de Physique Théorique, CEA Saclay

The decoding of several topological quantum codes (TQC) can be mapped onto statistical physics models (SPM). This mapping relates the successful decoding of the error syndrome of the TQC to a certain phase of the respective SPM. The error-correction performance of several TQC-s have been analyzed using Monte Carlo (MC) simulations of the corresponding SPM. We, on the other hand, use high-temperature series expansion (HTSE) to analyze the decoding performance of the toric code. In contrast to zero temperature simulations, which estimate the threshold of the minimum-weight perfect-matching decoder, our method naturally provides an estimate of that of the maximum-likelihood decoder. First, we analyze the full phase diagram of the 2D random-bond Ising model by computing HTSE to a higher order than previously performed. From our analysis, we estimate the accuracy threshold of the toric code in absence of measurement imperfections. We compare our result to those obtained by MC simulations and network model analysis. Then, we perform HTSE of the zero-field free-energy and the Wilson loop order parameter in the 3D Ising gauge theory in the presence of quenched disorder. The latter model describes the decoding of the toric code subject to measurement errors.

CPP 69.6 Fri 11:15 H19

Local and translational dynamics of water in various confinements investigated via ^{1}H and ^{2}H NMR — •Simon Schoner, Max Weigler, and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstr. 6, 64289, Darmstadt, Germany

Confined water is interesting for several reasons. On the one hand the topic is highly relevant in biology or geology where water is often found in soft or hard confinements, water around proteins or in rods being prime examples. On the other hand confined water allows one to investigate liquid water at low temperatures, where normally crystallization would occur, and, in this way, to obtain insights into the heavily debated glass transition of water. We investigate the dynamics of water confined in various rigid matrices using ^{1}H and ^{2}H NMR experiments. One goal is to obtain information on the influence of different kinds of confinements and pore sizes on the self diffusion and the structural relaxation of water. Especially, we address the question whether translational diffusion and local reorientation are affected by confinement in a comparable way. First measurements with D_2O and H_2O indicate similar correlation times and diffusion coefficients for both MCM-48 and MCM-41 confinements with comparable pore sizes between 2 and 3 nm.

CPP 69.7 Fri 11:30 H19

Universal hidden order in amorphous cellular geometries — •Gerd E Schröder-Turk — Murdoch University, Perth, School of Engineering and IT, WA 6150, Murdoch, Australia

Partitioning space into cells is central to many fields of science and technology, as well as to resource distribution problems in economics and telecommunication. The nature of cellular partitions is often defined by optimization with respect to certain properties, such as interface area in the Kelvin problem, packing density in the Kepler problem, or cell centrality in the Quantizer problem. In all known cases, the optimal solutions are crystalline configurations with long range order. To date, no optimization problem has been identified where the optimal solution is a disordered configuration. Amorphous, or disordered, structures are generally considered to be intermittent meta-stable states that prevent the system from attaining the optimal ordered structures. Here we use Lloyd's iteration to demonstrate the existence and stability of a special disordered state in the three-dimensional Quantizer problem, despite the existence of lower-energy crystalline configurations. Akin to a thermodynamic phase, this state is universal. Specifically, irrespective of the level and type of disorder in the initial configurations, we find a convergence to the same amorphous state, representing configurations characterized by the same structure factor and energy distributions. This highly degenerate state is characterised by an anomalous suppression of long-wavelength density fluctuations, known as hyperuniformity.

CPP 70: Closing talk (joint session BP/CPP/DY)

Time: Friday 12:30–13:15 Location: H1

Invited Talk CPP 70.1 Fri 12:30 H1

Pattern formation in active cytoskeletal systems — •Andreas R. Bausch — Lehrstuhl für Biophysik, Technische Universität München, 85747 Garching

Living cells rely on the self-organization mechanisms of cytoskeleton to adapt to their requirements. In processes such as cell division, or cellular motility rely on the controlled self-assembly and disassembly of well defined active cytoskeletal structures interacting with lipid membranes. One important and promising strategy to identify the underlying governing principles is to quantify the underlying physical processes in model systems mimicking functional units of living cell. Here I*ll present in vitro minimal model systems consisting of active microtubule and actin filament systems which show pattern formation resulting from active transport processes. I will discuss how small variations in local interactions results in nematic or polar patterns in high density motility essays. With the example of reconstituted active vesicles I will discuss how to relate local force exertion and tension generation to shape transformations, blebbing, invagination or tethering of lipid membranes