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Overview of Invited Talks and Sessions

(Lecture halls GÖR 226, MER 02, and ZEU 255; Poster P3 and P1A)

Invited Talks

CPP 1.1	Mon	9:30–10:00	GÖR 226	**Strategies for advancing the performance of organic photovoltaics** — •Thomas Anthopoulos
CPP 1.7	Mon	11:30–12:00	GÖR 226	**Lost in translation? Transport resistance in organic solar cells** — •Carsten Deibel
CPP 2.1	Mon	9:30–10:00	MER 02	**Molecular Theories meet Explainable Machine Learning – Novel Concepts for Advanced Drug Formulations** — •Jens Smiatek
CPP 11.1	Mon	15:00–15:30	GÖR 226	**Quantifying the potential of organic solar cells using luminescence measurements and modelling** — •Jenny Nelson
CPP 12.1	Mon	15:00–15:30	MER 02	**Adaptive Resolution Simulations: Past, Present and Open (Boundaries) Future** — Luis A. Baptista, Mauricio Sevilla, Kurt Kremer, •Robinson Cortes-Huerto
CPP 13.1	Mon	15:00–15:30	ZEU 255	**Nanocomposites and polymer thin films: from gas phase synthesis to functional applications** — •Franz Faupel, Stefan Schröder, Alexander Vahl, Salih Veziroglu, Cenk Aktas, Thomas Strunskus
CPP 19.1	Tue	9:30–10:00	MER 02	**Multiscale Model of Flow-Induced Crystallization in Polymers** — David Nicholson, Marat Andreev, Chenmay Gangal, •Gregory Rutledge
CPP 20.1	Tue	9:30–10:00	ZEU 255	**Granular Matter Rheology – fluid-/solid-like behavior and state-transitions** — •Stefan Luding
CPP 29.1	Wed	9:30–10:00	MER 02	**Imaging mineral-water interfaces with atomic force microscopy** — •Angelika Kühnle
CPP 53.1	Thu	15:00–15:30	ZEU 255	**Aqueous nanoclusters govern ionic transport in dense polymer membranes** — •Joachim Dzubiella
CPP 56.1	Fri	9:30–10:00	GÖR 226	**Self-assembled optical metamaterials** — •Ullrich Steiner
CPP 56.7	Fri	11:30–12:00	GÖR 226	**Simulating quantum systems with plasmonic waveguide arrays** — •Stefan Linden
CPP 56.8	Fri	12:00–12:30	GÖR 226	**single molecule detection on a smartphone microscope enabled by DNA origami biosensors** — •Philip Tinnefeld
CPP 57.1	Fri	9:30–10:00	MER 02	**Chiral transport of active and passive colloids** — •Anke Lindner, Andreas Zöttl, Olivia du Roure, Eric Clement, Francesca Tesser, Guangying Jing
CPP 58.1	Fri	9:30–10:00	ZEU 255	**Studies of polymer thermosets using scattering techniques** — •Mats Johansson

Invited Talks of the joint Symposium SKM Dissertation Prize 2023 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ 04	**Diffusion of antibodies in solution: from individual proteins to phase separation domains** — •Anita Girelli
SYSD 1.2	Mon	10:00–10:30	HSZ 04	**Intermediate Filament Mechanics Across Scales** — •Anna V. Schepers

SYSD 1.3	Mon	10:30–11:00	HSZ 04	**Ultrafast Probing and Coherent Vibrational Control of a Surface Structural Phase Transition** — •Jan Gerrit Horstmann
SYSD 1.4	Mon	11:00–11:30	HSZ 04	**Electro-active metasurfaces employing metal-to-insulator phase transitions** — •Julian Karst
SYSD 1.5	Mon	11:30–12:00	HSZ 04	**The role of unconventional symmetries in the dynamics of many-body systems** — •Pablo Sala

Invited Talks of the joint Symposium Physics of Fluctuating Paths (SYFP)

See SYFP for the full program of the symposium.

SYFP 1.1	Tue	9:30–10:00	HSZ 01	**Time at which a stochastic process achieves its maximum** — •Satya Majumdar
SYFP 1.2	Tue	10:00–10:30	HSZ 01	**Fluctuations and molecule-spanning dynamics of single Hsp90 proteins on timescales from nanoseconds to days** — •Thorsten Hugel
SYFP 1.3	Tue	10:30–11:00	HSZ 01	**Path reweighting for Langevin dynamics** — •Bettina Keller
SYFP 1.4	Tue	11:15–11:45	HSZ 01	**Out-of-equilibrium dynamics of trapped Brownian particles** — •Raul A. Rica
SYFP 1.5	Tue	11:45–12:15	HSZ 01	**Thermodynamics of Clocks** — •Patrick Pietzonka

Sessions

CPP 1.1–1.11	Mon	9:30–13:00	GÖR 226	**Focus: Organic Solar Cells Based on Non-fullerene Acceptors: Loss Mechanism and Options for Above 20 % Efficiencies I**
CPP 2.1–2.12	Mon	9:30–13:00	MER 02	**Modeling and Simulation of Soft Matter I**
CPP 3.1–3.4	Mon	9:30–10:30	ZEU 255	**Hydrogels and Microgels**
CPP 4.1–4.12	Mon	9:30–13:00	TOE 317	**Active Matter I (joint session BP/CPP/DY)**
CPP 5.1–5.10	Mon	9:30–12:30	POT 81	**2D Materials I (joint session HL/CPP)**
CPP 6.1–6.10	Mon	9:30–12:30	POT 251	**Perovskite and photovoltaics I (joint session HL/CPP)**
CPP 7.1–7.6	Mon	9:30–11:15	POT 361	**Organic Semiconductors (joint session HL/CPP)**
CPP 8.1–8.8	Mon	10:45–13:00	ZEU 255	**Responsive and Adaptive Systems**
CPP 9.1–9.5	Mon	11:30–12:45	SCH A 315	**Organic Thin Films, Organic-Inorganic Interfaces (joint session DS/CPP)**
CPP 10.1–10.3	Mon	14:30–15:30	POT 106	**Instrumentation and Methods for Micro- and Nanoanalysis (joint session KFM/CPP)**
CPP 11.1–11.7	Mon	15:00–17:15	GÖR 226	**Focus: Organic Solar Cells Based on Non-fullerene Acceptors: Loss Mechanism and Options for Above 20 % Efficiencies II**
CPP 12.1–12.7	Mon	15:00–17:15	MER 02	**Modeling and Simulation of Soft Matter II**
CPP 13.1–13.10	Mon	15:00–18:00	ZEU 255	**Composites and Functional Polymer Hybrids**
CPP 14.1–14.11	Mon	15:00–18:15	ZEU 160	**Active Matter II (joint session DY/BP/CPP)**
CPP 15.1–15.10	Mon	15:00–18:15	POT 81	**2D Materials II (joint session HL/CPP)**
CPP 16.1–16.11	Mon	15:00–17:45	GER 39	**Nanostructures at Surfaces (joint session O/CPP)**
CPP 17.1–17.60	Mon	18:00–20:00	P3	**Poster Session I**
CPP 18.1–18.13	Tue	9:30–13:00	GÖR 226	**Organic Electronics and Photovoltaics I (joint session CPP/HL)**
CPP 19.1–19.12	Tue	9:30–13:00	MER 02	**Crystallization, Nucleation and Self-Assembly**
CPP 20.1–20.10	Tue	9:30–12:30	ZEU 255	**Polymer and Molecular Dynamics, Friction and Rheology**
CPP 21.1–21.11	Tue	9:30–12:30	TOE 317	**Active Matter III (joint session BP/CPP/DY)**
CPP 22.1–22.10	Tue	9:30–12:15	POT 81	**2D Materials III (joint session HL/CPP)**
CPP 23.1–23.12	Tue	9:30–13:00	POT 112	**Optical Properties (joint session HL/CPP)**
CPP 24.1–24.11	Tue	10:00–13:00	MOL 213	**Complex Fluids and Soft Matter I (joint session DY/CPP)**
CPP 25.1–25.4	Tue	12:00–13:00	HSZ 201	**Molecular Electronics and Photonics (joint session TT/CPP)**
CPP 26.1–26.3	Tue	14:00–14:45	MER 02	**Electrical, Dielectrical and Optical Properties of Thin Films**
CPP 27.1–27.4	Tue	14:00–15:00	ZEU 147	**Glasses and Glass Transition I (joint session DY/CPP)**
CPP 28.1–28.11	Wed	9:30–12:30	GÖR 226	**Molecular Electronics and Excited State Properties (joint session CPP/TT)**
CPP 29.1–29.11	Wed	9:30–12:45	MER 02	**Interfaces and Thin Films**

CPP 30.1–30.12	Wed	9:30–13:00	TOE 317	**Biopolymers and Biomaterials I (joint session BP/CPP)**
CPP 31.1–31.10	Wed	9:30–13:00	ZEU 160	**Focus Session: From Inter-individual Variability to Heterogeneous Group Dynamics and Disorder in Active Matter (joint session DY/BP/CPP)**
CPP 32.1–32.10	Wed	9:30–12:30	POT 81	**2D Materials IV (joint session HL/CPP)**
CPP 33.1–33.11	Wed	9:30–13:00	POT 251	**Perovskite and photovoltaics II (joint session HL/CPP)**
CPP 34.1–34.11	Wed	10:00–13:00	ZEU 147	**Wetting, Droplets and Microfluidics I (joint session DY/CPP)**
CPP 35.1–35.66	Wed	11:00–13:00	P1	**Poster Session II**
CPP 36.1–36.9	Wed	15:00–17:30	GÖR 226	**Organic Electronics and Photovoltaics II (joint session CPP/HL)**
CPP 37.1–37.5	Wed	15:00–16:15	MER 02	**Nanostructures, Nanostructuring and Nanosized Soft Matter**
CPP 38.1–38.12	Wed	15:00–18:15	MOL 213	**Microswimmers and Fluid Physics of Life (joint session DY/CPP)**
CPP 39.1–39.12	Wed	15:00–18:15	ZEU 160	**Focus Session: Physics of Fluctuating Paths (joint session DY/CPP)**
CPP 40.1–40.10	Wed	15:00–17:30	GER 37	**2D Materials V: Growth, Structure and Substrate Interaction (joint session O/CPP)**
CPP 41.1–41.6	Wed	16:30–18:00	MER 02	**Biopolymers, Biomaterials and Bioinspired Functional Materials II (joint session CPP/BP)**
CPP 42.1–42.10	Thu	9:00–12:35	POT 51	**Battery Materials (joint session KFM/CPP)**
CPP 43.1–43.11	Thu	9:30–12:30	GÖR 226	**Organic Electronics and Photovoltaics III (joint session CPP/HL)**
CPP 44.1–44.13	Thu	9:30–13:00	MER 02	**Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)**
CPP 45.1–45.9	Thu	9:30–12:00	ZEU 255	**Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods**
CPP 46.1–46.12	Thu	9:30–13:00	ZEU 160	**Active Matter IV (joint session DY/BP/CPP)**
CPP 47.1–47.9	Thu	9:30–12:00	POT 81	**2D Materials VI (joint session HL/CPP)**
CPP 48.1–48.11	Thu	10:15–13:15	SCH A 251	**Data Driven Materials Science: Big Data and Work Flows – Microstructure-Property-Relationships (joint session MM/CPP)**
CPP 49.1–49.9	Thu	10:30–12:45	GER 37	**2D Materials VII: Heterostructures (joint session O/CPP)**
CPP 50.1–50.3	Thu	12:15–13:00	ZEU 255	**Glasses and Glas Transition II**
CPP 51.1–51.8	Thu	15:00–17:15	GÖR 226	**Hybrid and Perovskite Photovoltaics III**
CPP 52.1–52.5	Thu	15:00–16:15	MER 02	**Wetting, Fluidics and Liquids at Interfaces and Surfaces III (joint session CPP/DY)**
CPP 53.1–53.9	Thu	15:00–17:45	ZEU 255	**Charged Soft Matter, Polyelectrolytes and Ionic Liquid**
CPP 54.1–54.5	Thu	16:30–17:45	MER 02	**2D Materials VIII**
CPP 55	Thu	18:00–19:00	MER 02	**Members' Assembly**
CPP 56.1–56.8	Fri	9:30–12:30	GÖR 226	**Focus: Self-Assembly of Plasmonic Nanostructures (joint session CPP/HL)**
CPP 57.1–57.12	Fri	9:30–13:00	MER 02	**Complex Fluids and Colloids, Micelles and Vesicles II (joint session CPP/DY)**
CPP 58.1–58.7	Fri	9:30–11:30	ZEU 255	**Polymer Networks and Elastomers**
CPP 59.1–59.8	Fri	9:30–12:00	TOE 317	**Active Matter V (joint session BP/CPP/DY)**
CPP 60.1–60.1	Fri	12:15–13:00	HSZ 03	**Closing Plenary Talk (joint session BP/CPP)**

Members' Assembly of the Chemical and Polymer Physics Division

Thursday 18:00-19:00 MER 02

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

CPP 1: Focus: Organic Solar Cells Based on Non-fullerene Acceptors: Loss Mechanism and Options for Above 20 % Efficiencies I

Organized by Dieter Neher and Christoph J. Brabec

Time: Monday 9:30–13:00 Location: GÖR 226

Invited Talk CPP 1.1 Mon 9:30 GÖR 226

Strategies for advancing the performance of organic photovoltaics — •Thomas Anthopoulos — King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia

The dramatic advances in the power conversion efficiency (PCE) of organic photovoltaics (OPVs) witnessed in recent years have been primarily driven by the development of new materials and the minimisation of performance losses associated with conventional cell architectures. This talk will discuss our recent OPV work, focusing on practical strategies for boosting cell performance. I will first discuss using low-dimensional charge-extracting interlayers and the numerous advantages of these innovative materials for next-generation OPVs. I will then present recent progress in using molecular dopants to improve the PCE of OPVs and how their combination with innovative interlayers can improve the material utilisation and circularity of the ensuing OPV cells without compromising their performance.

CPP 1.2 Mon 10:00 GÖR 226

Can Organic Solar Cells Beat the Near-Equilibrium Thermodynamic Limit? — Tanvi Upreti[1], •Constantin Tormann[2], and Martijn Kemerink[1,2] — [1]Complex Materials and Devices, Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden — [2]Insitute for Molecular Systems Engineering and Advanced Materials, Heidelberg University, Germany

Switching to non-fullerene acceptors has led to an impressive increase in power conversion efficiencies (PCEs) of organic photovoltaic cells over the past decade. Despite this, the PCE of such devices is still below the near-equilibrium limit of the corresponding material, which is particularly evident from losses in the open-circuit voltage (Voc). A prominent yet incompletely understood loss channel affecting Voc is the thermalization of photogenerated charge carriers in the density of states, which is broadened by energetic disorder. In contrast to symmetric morphologies like classic bulk heterojunctions, morphologies with a gradient in the donor:acceptor ratio can mitigate this loss channel by rectifying the diffusive motion of the thermalizing photogenerated charge carriers. Here, we show by extensive numerical modelling how funnel-shaped donor and acceptor-rich domains in a phase-separated morphology promote directed transport of positive and negative charge carriers towards the anode and cathode, respectively. In such optimized funnel morphologies, this kinetic, nonequilibrium effect even allows one to surpass the near-equilibrium thermodynamic limit for the same active material in the absence of gradients.

CPP 1.3 Mon 10:15 GÖR 226

Transparent Conductive Electrodes: Figure of Merit Revisited for Photovoltaics — •Harald Hoppe — Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany — Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstrasse 10, 07743 Jena, Germany

Figure of Merits (FOMs) are meant to provide a simple means for assessing the suitability of a certain material for or compartments within devices in general. In case of photovoltaic devices, the role of the transparent conductive electrode is to allow as much as possible light to enter into the device as well as to enable current flow out of the device. Over the last 5 decades a number of FOMs were introduced based on several approaches. Here we present a rather novel, yet implicit approach for an FOM, which is highly suitable for photovoltaics, allowing to assess the potential photovoltaic performance quantitatively.

CPP 1.4 Mon 10:30 GÖR 226

Reconnoitering the impact of fluorination on both donor and non-fullerene acceptor in bulk heterojunction organic photovoltaics — •Shahidul Alam[1], Jafar I. Khan[1], Vojtech Nádaždy[3], Tomáš Váry[3], Aurelien D. Sokeng[2], Md Moidul Islam[2], Christian Friebe[2], Wejdan Althobaiti[2], Martin Hager[2], Ulrich S. Schubert[2], Carsten Deibel[4], Denis Andrienko[5], Frédéric Laquai[1], and Harald Hoppe[2] — [1]KAUST Solar Center (KSC), Kingdom of Saudi Arabia — [2]FSU Jena, Germany — [3]Slovak Academy of Sciences, Bratislava — [4]TU Chemnitz, Germany — [5]MPIP, Mainz, Germany

Organic solar cells' performance can be often effectively improved through fluorination of the donor and/or non-fullerene acceptor (NFA). The end-group fluorination of the well-known NFA ITIC yields further extension of the absorption spectrum to the near infrared, which results in an increment of the device's photocurrent as compared to the non-fluorinated version. Herein, ITIC and two fluorinated variants of ITIC (ITIC-2F* and ITIC-4F) were synthesized and systematically investigated the influence of end-group fluorination physicochemical properties, optical properties, and photovoltaic performance. Photovoltaic parameters are discussed in terms of exciton quenching, charge generation, charge dissociation, and recombination losses. Specifically, it is found that fluorinated acceptors control the devices' open circuit voltage. All the results shed light on the importance of the energy landscape and the quadrupole moment of acceptor beyond the underlying donor-acceptor interface.

CPP 1.5 Mon 10:45 GÖR 226

Synthesis and Characterization of Organic Heterojunction Model Interfaces — •Hanbo Yang[1], Jarvist Moore Frost[1], Jenny Nelson[1], and Hugo Bronstein[2] — [1]Imperial College London, London, UK — [2]Cambridge University, Cambridge, UK

Control of the molecular configuration at the interface of an organic heterojunction is key to the development of efficient optoelectronic devices. Due to the difficulty in characterizing these buried and (likely) disordered heterointerfaces the interfacial structure in most systems remains a mystery. Here, we demonstrate a novel synthetic strategy to design and control model interfaces, allowing for their detailed study in isolation from the bulk material. This is achieved by the synthesis of a donor polymer-non-fullerene acceptor 'through space' linked system, where the exact position and orientation of the moieties is completely controlled and we furthered showed that the kinetics of charge separation can be tuned using transient absorption spectroscopy and excited state calculations.

CPP 1.6 Mon 11:00 GÖR 226

Direct Determination of the Photogenerated Free Charge Carrier Luminescence in Organic Solar Cells via Transient Photoluminescence Measurements — •Jared Faisst, Mathias List, and Uli Würfel — Fraunhofer ISE, Freiburg, Deutschland

Photoluminescence (PL) measurements have shown to be a valuable tool characterizing the optoelectronic properties of semiconductors. In organic solar cells, the PL measurement of free charge carriers is hindered by the strong and spectrally broad luminescence of non-dissociated local exciton recombination. Therefore, the PL of free charge carriers under steady state condition is not directly detectable. To overcome this problem, we make use of the vastly different lifetimes of local excitons (ps-ns) and free charge carriers (μs). In this work, we present experimental time resolved PL data of a fullerene based D18:$PC_{71}BM$ and two non-fullerene based D18:Y6 and PV-X plus organic solar cells and demonstrate the possibility to separate the luminescence of local excitons from the one of free charge carriers. We further show that the luminescence of the free charge carriers indeed correlates with the quasi-Fermi level splitting as expected. Hence, this novel measurement technique eventually allows to investigate free charge carriers in organic absorber layers directly. This is of great importance to further understand recombination mechanisms and degradation effects and to identify optimization potentials.

15 min. break

Invited Talk CPP 1.7 Mon 11:30 GÖR 226

Lost in translation? Transport resistance in organic solar cells — •Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

With the advent of non-fullerene acceptors, breaking the 20 % power conversion efficiency limit is within close reach for organic solar cells. Understanding the efficiency-limiting processes remains important.

I will discuss how losses in the fill factor can be due to the transport resistance, a voltage loss because of a low conductivity in the active layer. Its relevance for organic solar cells was only shown a half dozen years ago [1]. I will present transport resistance limiting different organic solar cell types, and then focus on fresh and thermally degraded PM6:Y6 solar cells (heated to 85°C, in the dark, under nitrogen atmosphere), a state-of-the-art system based on the non-fullerene Y6. The increasing fill factor losses on this degradation path are because of the transport resistance [2]. The reason seems to be trap formation in the tail states, which decrease the active layer conductivity.

[1] U. Würfel, D. Neher, A. Spies, S. Albrecht, Nat. Commun. 6, 6951 (2015).

[2] C. Wöpke, C. Göhler, M. Saladina, X. Du, L. Nian, C. Greve, C. Zhu, K. M. Yallum, Y. J. Hofstetter, D. Becker-Koch, N. Li, T. Heumüller, I. Milekhin, D. R. T. Zahn, C. J. Brabec, N. Banerji, Y. Vaynzof, E. M. Herzig, R. C. I. MacKenzie, C. Deibel. Nat. Commun. 13, 3786 (2022).

CPP 1.8 Mon 12:00 GÖR 226

Thermal Degradation Mechanism in PM6: Y-series Acceptors Organic Solar Cells

— •Si Chen, Julien Gorenflot, and Laquai Frederic — Abdullah University of Science and Technology Thuwal 23955-6900, Saudi Arabia

The stability issue is the core restriction for the application of organic solar cells (OSCs), and the study of the degradation mechanism of high-efficient PM6: Y-series systems is an urgent problem to be solved. We concluded one specific pathway of FF degradation for typical PM6:Y-series acceptors organic solar cells since FF changed most obviously after thermal aging. After developing several characterization measurements, including time-delayed collection field (TDCF), light intensity dependent measurements, etc. to study the photophysics of PM6:Y-series solar cells before and after thermal degradation, we can quantify FF degradation with field-dependent charge generation, non-geminate recombination, and transport resistance factors. The effect of transport resistance is quantified by the Suns-Voc method. The results show that the increase of charge transport resistance is the primary factor leading to FF degradation, which can be further explained by excessive phase separation with the information from GIWAXS and AFM. Our work can not only provide material design ideas for highly efficient and stable organic solar cells by figuring out the thermal degradation mechanism of PM6:Y-series organic solar cells but also come up with a new methodology to quantify the FF degradation of organic solar cells.

CPP 1.9 Mon 12:15 GÖR 226

Photophysics of Poly(3-hexylthiophene):Non-Fullerene Acceptor Based Organic Solar Cells

— •Wejdan Althobaiti, Jafar Khan, Julien Gorenflot, Shahidul Alam, George Harrison, Stefaan De Wolf, and Frédéric Laquai — King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Physical Sciences and Engineering Division (PSE), Saudi Arabia

Charge generation can proceed through two different paths in Bulk Heterojunction based organic solar cells which are electron transfer from donor to acceptor and hole transfer from acceptor to donor. These processes can be controlled by Electron Affinity (EA) offsets and Ionization Energy (IE) offsets, respectively. Understanding the relationship between the IE offsets, EA offsets between donor and acceptor materials, and the performance of OSCs could improve the charge generation efficiency. We characterized the impact of large IE and EA offsets on device performances and more precisely on the internal quantum efficiency (IQE) using a wide bandgap polymer donor which has shallow IE such as P3HT and Non Fullerene Acceptor (NFA). This provides a wide range of diagonal bandgap (IE of the donor and EA of the acceptor). Thus, enables us to find the relation between small diagonal bandgap and the decrease of the IQE in energy gap law framework. Low IQE while high exciton quenching observed can be explained due to charge recombination as our results demonstrated by geminate and non-geminate recombination.

CPP 1.10 Mon 12:30 GÖR 226

Efficient Nanoscale Exciton Transport in Non-fullerene Organic Solar Cells Enables Reduced Bimolecular Recombination of Free Charges

— •Drew B. Riley[1], Oskar J. Sandberg[1], Nasim Zarrabi[1], Ryun Kim[2], Paul Meredith[1], and Ardalan Armin[1] — [1]Swansea Univeristy, Swansea, Wales. — [2]Cambridge Univeristy, Cambridge, UK

The origins of reduced bimolecular recombination in high efficiency OPV-based solar cells are debated, and mechanisms related to the charge-transfer (CT) state and free-carrier encounter dynamics have been proposed as underlying factors.[1] Further, it is expected that the CT-state dynamics is strongly influenced by exciton dynamics in low off-set blends.[2]

In this presentation I will explore the role exciton dynamics play in the charge generation and recombination processes. Specifically, I will introduce a photoluminescence-based probe to quantify the acceptor domain size in OPV blends. It will be shown that NFA-based blends form larger domains than fullerene-based systems but that this increase is unable to account for the observed non-Langevin recombination. Further, I will show that the reduction of bimolecular recombination is correlated with enhanced exciton dynamics within the NFA domains. This indicates that the processes responsible for efficient exciton transport also enable strongly non-Langevin recombination in high efficiency NFA-based solar cells with low energy offsets.

[1] A. Armin, et.al. AEM, 11, 2003570, 2021.

[2] A. Classen,et.al. Nat.Energy, 5,2020.

CPP 1.11 Mon 12:45 GÖR 226

Power-law density of states in organic solar cells revealed by the open-circuit voltage dependence of the ideality factor

— •Maria Saladina[1], Christopher Wöpke[1], Clemens Göhler[1], Ivan Ramirez[2], Olga Gerdes[2], Chao Liu[3,4], Ning Li[3,4,5], Thomas Heumüller[3,4], Christoph J. Brabec[3,4], Karsten Walzer[2], Martin Pfeiffer[2], and Carsten Deibel[1] — [1]Technische Universität Chemnitz, Germany — [2]Heliatek GmbH, Germany — [3]FAU Erlangen-Nürnberg, Germany — [4]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Germany — [5]South China University of Technology, China

We determine the density of states (DOS) in disordered semiconductors via the diode ideality factor (n_{id}). We employ illumination intensity and temperature-dependent open-circuit voltage measurements. In amorphous silicon, we found that n_{id} only depends on the temperature, and can be explained by an exponential DOS distribution.

For the organic donor-acceptor solar cells, we find that n_{id} is not only temperature but also light intensity-dependent. The seemingly unsystematic dependence of n_{id} on the light intensity becomes systematic once the former is displayed in dependence of the open-circuit voltage, which is a means to sample the DOS distribution at a certain energetic depth. This evaluation approach leads to our central result: the DOS follows a power-law distribution over a broad range of energies. In particular, for the investigated organic solar cells under working conditions the DOS is best represented by the power-law, not a gaussian or exponential one.

CPP 2: Modeling and Simulation of Soft Matter I

Time: Monday 9:30–13:00 Location: MER 02

Invited Talk CPP 2.1 Mon 9:30 MER 02

Molecular Theories meet Explainable Machine Learning – Novel Concepts for Advanced Drug Formulations — •Jens Smiatek — Institute for Computational Physics, University of Stuttgart, Germany — Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach (Riss), Germany

Pharmaceutical processes and drug formulations are based on a variety of molecular mechanisms and principles. Significant advances have been made in recent years in terms of basic understanding. Despite these advances, a large number of mechanisms are not yet fully understood, which would be of great advantage, especially for the optimization of development processes as well as the quality and stability of drugs. In this talk I will present fundamental molecular theories of electronic interactions in solutions. Due to the large number of components and the complexity of the interactions, these theories can only be used for a qualitative understanding. However, by combining it with explainable machine learning, the basic molecular mechanisms can be identified and the corresponding thermodynamic properties of the solutions can be predicted. I will present some examples and discuss the underlying benefits and additional challenges for future developments.

CPP 2.2 Mon 10:00 MER 02

Revealing the relation between structure and dynamics using unsupervised machine learning — •Moumita Maiti[1], Anand Narayanan Krishnamoorthy[2], Youssef Mabrouk[2], Diddo Diddens[2], and Andreas Heuer[1] — [1]Institute of Physical Chemistry, University of Münster, Corrensstrasse 28/30, 48149 Münster, Germany — [2]Forschungszentrum Jülich GmbH, Helmholtz-Institute Münster (IEK-12), Corrensstraße 46, 48149 Münster, Germany

Molecular dynamics trajectories of Li-ions in electrolytes with different anions are analysed using an unsupervised machine learning algorithm to understand the relation between structure and dynamics. The trajectories are generated using a polarizable force-field model instead of the standard OPLS force-field, thereby generating excellent agreement of structural and dynamical properties with experiment. The high-dimensional feature space is constructed from the distances and angles between Li-ions and its neighbours, reflecting the structural information of local environments. It can be reasonably reduced to 2 dimensions using the dimension reduction algorithm umap. This is performed for a large number of Li-ions. After the mapping distinct clusters can be identified. Although they are based on structural properites, they also reflect different dynamical properties with respect to diffusivity and ion-correlations. We finally show how the total ionic conductivity can be expressed in terms of the structural information of the first solvation shell.

CPP 2.3 Mon 10:15 MER 02

Data reweighting in metadynamics simulations — Timo Schäfer[1] and •Giovanni Settanni[1,2] — [1]Department of Physics, Johannes-Gutenberg University Mainz, Germany — [2]Faculty of Physics and Astronomy, Ruhr University Bochum, Germany

The data collected along a metadynamics simulation can be used to recover information about the underlying unbiased system by means of a reweighting procedure. We analyze the behavior of several reweighting techniques in terms of the quality of the reconstruction of the underlying unbiased free energy landscape in the early stages of the simulation and propose a simple reweighting scheme that we relate to the other techniques. We show[1] that the free energy landscape reconstructed from reweighted data can be more accurate than the negative bias potential depending on the reweighting technique, the stage of the simulation, and the adoption of well-tempered or standard metadynamics. While none of the tested reweighting techniques from the literature provides the most accurate results in all the analyzed situations, the one proposed here, in addition to helping simplifying the reweighting procedure, converges quickly and precisely to the underlying free energy surface in all the considered cases, thus allowing for an efficient use of limited simulation data.

[1]Schäfer TM, Settanni G. J Chem Theory Comput. 2020 Apr 14;16(4):2042-2052. doi: 10.1021/acs.jctc.9b0086

CPP 2.4 Mon 10:30 MER 02

findR: An automatized workflow from molecular dynamic simulation to quantum chemical methods for reaction discovery — •Gunnar Schmitz[1], Özlem Yönder[2], Vanessa Angenent[3], Christof Hättig[2], and Rochus Schmid[3] — [1]Ruhr-Universität Bochum, Lehrstuhl für Theoretische Chemie II, Bochum, Germany, 44801 Bochum — [2]Ruhr-Universität Bochum, Lehrstuhl für Theoretische Chemie I, Bochum, Germany, 44801 Bochum — [3]Ruhr-Universität Bochum, Lehrstuhl für Anorganische Chemie II, Bochum, Germany, 44801 Bochum

Computer-guided reaction discovery is still an open issue, which will be vital for applications in science and industry. For this purpose, we present an automatized workflow that, starting from molecular dynamics simulations (MD), identifies reaction events based on graph theory, filters them, and prepares them for accurate quantum chemical calculations using e.g. Density Functional Theory (DFT) or Coupled Cluster methods. The capabilities of the automatized workflow are demonstrated by the example of simulations for the combustion of polycyclic aromatic hydrocarbons. A limiting factor of the reaction sampling by means of MD simulations is the required simulation time to observe reactions. In order to enhance this process, we compare different acceleration techniques like metadynamics and a nano reactor setup, in which a spherical confinement is combined with periodically applied forces directed to the simulation box center. We demonstrate that our workflow can be used to identify reactions without prior chemical knowledge and can give new insights into the combustion process.

CPP 2.5 Mon 10:45 MER 02

Data-driven analysis and prediction of the performance of cleansing solutions — •takahiro yokoyama[1], hideki miwake[2], ryouichi nakatake[2], noriyoshi arai[1], and arash nikoubashman[1,3] — [1]Department of Mechanical Engineering, Keio University, Yokohama, Japan — [2]Research Institute, Fancl Corporation, Yokohama, Japan — [3]Institute of Physics, JGU Mainz, Germany

Cleansing solutions are complex multi-component liquids, which are commonly used to wash excess sebum, dirt, and make-up cosmetics directly from the skin. Their formulations typically contain a large variety of ingredients, including surfactants, viscosity modifiers, and polyols to meet the desired product requirements, such as high skin compatibility, moisture retention, and long shelf life. The large number of different components makes it, however, challenging to understand and predict the physical properties of such cleansing solutions, since the majority of established theories have been developed for pure systems. Machine learning (ML) methods are promising methods to solve these kinds of problems, as they can reveal non-trivial trends and interactions between the various components. In this work, we predict the cleansing performance of a large number of formulations using various ML methods, such as random forest regression and (recurrent) neural networks. Although this work focuses primarily on cleansing solutions, the applied methodology should be transferable to predict the physical properties of other multi-component liquids as well.

CPP 2.6 Mon 11:00 MER 02

Multiscale Simulation Framework for the electromechanical behavior of PEDOT:PSS — Steffen Kampmann[1], Alexander Croy[2], •Arezoo Dianat[1], and Gianaurelio Cuniberti[1] — [1]Chair of Materials Science and Nanotechnology, Faculty of Mechanical Science and Engineering, TU Dresden, Dresden , Germany — [2]Chair of Theoretical Chemistry, Faculty of Chemistry and Earth Sciences, Friedrich Schiller University Jena, Jena , Germany

Functional mechanically resilient polymer films, such as poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), play an important role for strain gauges or organic light-emitting diode displays [1-3]. Typically, the respective material behavior results from an interplay of mechanisms across multiple scales. The modeling and simulation workflow presented here enables the generation of disordered polymers and the linking of their mechanical and their electronic properties from the atomistic to the microscopic scale. In particular, we focus on the relationship between deformation and conductivity by combining density functional tight binding calculations, molecular dynamics simulations, and finite element calculations. The in-situ processing, evaluation as well as the exchange of the generated data across the simulation methods is performed using a Python framework which provides a computationally efficient assessment of material properties at different scales. Exemplarily, we present results for a strain gauge based on PEDOT:PSS. [1] R. Luo, et al., Progress in Organic Coatings, 162, 106593 (2022) [2] M. Cinquino et al., JS: AMD, 7, 1,100394 (2022) [3] L. Liu, et al., Organic Electronics, 89, 106047 (2021)

15 min. break

CPP 2.7 Mon 11:30 MER 02

Differentiable simulation for Solar Power Plants and beyond — •Stefan Kesselheim[1], Max Pargmann[2], and Jan Ebert[1] — [1]Forschungszentrum Jülich — [2]German Aerospace Center (DLR)

In Solar Power Plants, temperatures sufficient for chemical processes or the generation of electrical power are created by reflecting sunlight with thousands of mirrors ("heliostats") to a surface ("the receiver"). In operation, the temperature distribution on the receiver is critical for the performance and must be optimized. The heliostats are never perfectly flat as due to budget constraints, the construction is not optimal. We have devised a method to infer the heliostat surface from the reflection of the sun. The technique is based on an implementation of a simulation in PyTorch, where the automatic differentiation engine is used to optimize the surface. The surface is modeled as by a Non-Uniform Rational B-Spline (NURBS) and the NURBS parameters are subject to optimization. Furthermore we employ a regularization technique to mitigate the appearing challenge of ambiguous solutions. Our approach makes efficient use of GPUs based on PyTorch's linear algebra engine. We believe our approach poses an interesting example of a fruitful interaction of techniques originating from Machine Learning and simulation, that can serve as an exciting example how to integrate simulation and experimental data, for example in biomolecular simulation.

CPP 2.8 Mon 11:45 MER 02

Simulation-based inference of single-molecule force-spectroscopy — •Roberto Covino[1,2], Lars Dingeldein[1], and Pilar Cossio[3] — [1]Frankfurt Institute for Advanced Studies, 60438 Frankfurt am Main, Germany — [2]International Max Planck Research School on Cellular Biophysics, 60438 Frankfurt am Main, Germany — [3]Center for Computational Mathematics and Biology, Flatiron Institute, 10010 New York, United States

Single-molecule force spectroscopy (smFS) is a powerful approach to studying molecular self-organization. However, the coupling of the molecule with the ever-present experimental device introduces artifacts, that complicates the interpretation of these experiments. Performing statistical inference to learn hidden molecular properties is challenging because these measurements produce non-Markovian time series, and even minimal models lead to intractable likelihoods. To overcome these challenges, we developed a computational framework built on novel statistical methods called simulation-based inference (SBI). SBI enabled us to directly estimate the Bayesian posterior, and extract reduced quantitative models from smFS, by encoding a mechanistic model into a simulator in combination with probabilistic deep learning. Using synthetic data, we could systematically disentangle the measurement of hidden molecular properties from experimental artifacts. The integration of physical models with machine-learning density estimation is general, transparent, easy to use, and broadly applicable to other types of biophysical experiments.

CPP 2.9 Mon 12:00 MER 02

Coarse-grained modelling of liquid-liquid and liquid-gas interfaces — •Jakob Filser[1], Harald Oberhofer[2], Christoph Scheurer[1], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Chair for Theoretical Physics VII, University of Bayreuth

Modelling of dielectric interfaces remains a central challenge in computational chemistry. We present a new method to incorporate solvation effects into density-functional theory calculations of organic adsorbates at liquid-liquid and liquid-gas interfaces.

Simulating a large number of solvent molecules explicitly at first-principles level is generally not computationally tractable. We therefore resort to an implicit solvation approach, treating the solvent as a structureless dielectric continuum. Specifically, we advance the multipole-expansion method, in which we model the interface as the boundary of two semi-infinite media with different permittivity. Gauging the limiting behaviour for moving the solute from one bulk medium into the other is straightforward by referencing experimental transfer free energies. Complementary force-field level MD simulations with explicit solvent molecules are used as a reference for the behaviour at the interface. These calculations yield thermal distributions at atomic scale resolution, allowing for a fine assessment of the role of the solvent structure in the adsorption. In our implicit method, we employ a model for the transition of free energy terms, such as the surface tension, between the two media, aimed at reproducing the above mentioned thermal distributions extracted from an atomistic solvent model.

CPP 2.10 Mon 12:15 MER 02

Geometrical frustration causes self-limiting assembly in systems of bipods — •Aswathy Muttathukattil and Michael Engel — Institute for Multiscale Simulation, IZNF, Friedrich-Alexander Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Geometric frustration emerges in self-assembly if local interactions between building blocks are incompatible to form uniform (bulk) materials. Examples for geometrically frustrated assemblies with self-limiting size include protein filament bundles, twisted molecular crystals, bent core liquid-crystals and viral capsids. Despite of significant efforts to develop a general theory on geometrical frustration, it remains as a challenge to use it as a design principle to engineer finite-size equilibrium assemblies in soft matter. In this study, we control geometrical frustration deliberately and systematically in system of bipods to demonstrate self-limiting crystallization. Our minimal computational model consists of a central sphere that connect to two attractive rigid rods diametrically via a flexible hinge. Tuning the flexibility of the hinge and rod attraction, anisotropic fibrillar assemblies are observed. The fibrils do not grow wider than a fixed limit, which can be controlled by the misfit introduced by the radius of central sphere. Our model bipods can be realized in experiments as nanoparticles with tethered polymer bundles, partially unfolded polymer globules (including biopolymers like proteins) and organic molecules.

CPP 2.11 Mon 12:30 MER 02

Pair-Reaction Dynamics in Water: Competition of Memory, Potential-Shape and Inertial Effects — •Florian Brünig, Jan Daldrop, and Roland Netz — Freie Universität Berlin, Department of Physics, 14195 Berlin, Germany

When described by a one-dimensional reaction coordinate, pair-reaction rates in a solvent depend, in addition to the potential barrier height and the friction coefficient, on the potential shape, the effective mass and the friction relaxation spectrum, but a rate theory that accurately accounts for all these effects does not exist. We show how to extract all parameters of the generalized Langevin equation (GLE) and in particular the friction memory function from molecular dynamics (MD) simulations of two prototypical pair reactions in water, the dissociation of NaCl and of two methane molecules. Simulations of the GLE by Markovian embedding techniques accurately reproduce the pair-reaction kinetics from MD simulations without any fitting parameters, which confirms the accuracy of the approximative form of the GLE and of the parameter extraction techniques. By modification of the GLE parameters, we investigate the relative importance of memory, mass and potential-shape effects. Neglect of memory slows down NaCl and methane dissociation by roughly a factor of 2, neglect of mass accelerates reactions by a similar factor, the harmonic approximation of the potential shape gives rise to slight acceleration. This error cancellation explains why Kramers' theory, which neglects memory effects and treats the potential shape harmonically, describes reaction rates better than more sophisticated theories.

CPP 2.12 Mon 12:45 MER 02

The Crucial Role of Solvation Forces in the Steric Stabilization of Nanoplatelets — •Nanning Petersen, Martin Girard, Andreas Riedinger, and Omar Valsson — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz

The precipitation of ligand coated cadmium selenide nanoplatelets is linked to the formation of nanoplatelet stacks. The exact nature of nanoplatelets' interaction is an open question, as the van der Waals attraction is too weak to be the cause of stack formation. CdSe nanoplatelets combine a large facet to particle size ratio, and a very dense ligand shell. Both features are in favor of interactions in the form of solvation forces.

We use coarse-grained molecular dynamics simulations of ligand coated nanoplatelets in different alkane solvents to investigate the role of solvation forces in nanoplatelet interactions [1]. We demonstrate that solvation forces resulting from solvent layering are sufficiently strong to stabilize nanoplatelet stacks. We examine the dependence of solvation forces on the nanoplatelets' ligand shell, size, and other parameters. In particular, we demonstrate that for sufficiently large nanoplatelets, solvation forces are proportional to the interacting facet area. We show that their strength is intrinsically tied to the softness of the ligand shell, depends on the isomer of the alkane solvent, and is increasing with the alkane molecule length.

[1] N. Petersen, M. Girard, A, Riedinger, and O. Valsson, ChemRxiv, doi:10.26434/chemrxiv-2022-mw1cs-v3 (2022), accepted for publication in Nano Letters

CPP 3: Hydrogels and Microgels

Time: Monday 9:30–10:30 Location: ZEU 255

CPP 3.1 Mon 9:30 ZEU 255

Acousto-responsive poly(N-isopropylacrylamide) microgels — •Amin Rahimzadeh, Atieh Razavi, and Regine von Klitzing — Soft Matter at Interfaces, Department of Physics, Technical University of Darmstadt, Hochschulstraße 8, 64289 Darmstadt, Germany

In this work, we introduce a novel stimulus for Poly(N-isopropylacrylamide), known as PNIPAM, microgels. High-frequency ultrasonic waves provide the required energy for collapsing microgels while the solution temperature maintains below their volume phase transition temperature (VPTT). Ultrasound propagates through the liquid and its energy will be absorbed due to the liquid viscosity. A part of the energy will be absorbed due to the translational relaxation of the liquid molecules leading to the creation of a flow that is called acoustic streaming. Another part of the energy of the waves will be absorbed due to the rotational and vibrational relaxations of the liquid molecules. The former absorption is due to the dynamic viscosity and the latter is due to the bulk viscosity. We show that along with acoustic streaming, the absorbed energy due to the bulk viscosity provides the energy for breaking hydrogen bonds between the microgels and water molecules. The turbidity of the liquid is used as a way to visualize and quantify the energy absorption, by calculating the required energy for making the solution fully turbid. We use image processing to quantify the absorbed energy by the hydrogen bonds and investigate the effects of solution concentrations (0.2 wt.%, 1 wt.% and 5 wt.%), ultrasound amplitude and frequency.

CPP 3.2 Mon 9:45 ZEU 255

Swelling and nanophase separation of amphiphilic star polymer conetworks — •Reinhard Scholz and Michael Lang — Leibniz Institut für Polymerforschung, Hohe Str. 6, 01069 Dresden, Germany

Polymer conetworks consisting of complementary four functional stars coupled via complementary end groups are simulated within the framework of a lattice-based Monte Carlo algorithm. A classification of different stars reveals that the conetworks are dominated by ideal star configurations surrounded by four different bonding partners. In a good solvent, the simulation reproduces analytical scaling relations for swelling, modulus and residual bond orientation [1]. A selective solvent induces a phase separation between a swollen polymer phase and embedded clusters consisting of insoluble polymer stars. Due to the complementary end groups, all elastically active chains cross the phase boundary, so that residual bond orientations correspond either to swollen conformations, collapsed stars, or bonds across the phase boundary with a particularly large component along the interface normal. Calculated pair distributions and scattering functions reveal that the length scale of phase separation depends only weakly on the concentration over a broad range of concentrations, $c^* < c < 6c^*$.

[1] M. Lang, R. Scholz, L. Löser, C. Bunk, N. Fribiczer, S. Seiffert, F. Böhme, and K. Saalwächter, Macromolecules 55, 5997 - 6014 (2022).

CPP 3.3 Mon 10:00 ZEU 255

How topology impacts magnetic and rheological properties of a suspension of magnetic nanogels — •Ivan Novikau[1], Alla Dobroserdova[2], Ekaterina Novak[2], and Sofia Kantorovich[1,2] — [1]University of Vienna, Austria — [2]Ekaterinburg, Russia

Hydrogels are soft materials, that attracted solid interest over the last 6 decades and are widely used in chemical, biomedical, and even civil engineering applications. Today, at the front edge of gels' realm stand out nanogels, often additionally functionalization, for instance, by magnetic nanoparticles.

Given the magnetic nanogels (MNG's) size, typical time and velocity scales involved in their nanofluidics, experimental characterization of the systems is difficult. Here, we use molecular dynamics (MD) simulations in conjunction with the Lattice-Boltzmann (LB) scheme in order to describe how the MNG topology affects the rheological and magnetic properties of their suspensions.

We study in detail how the shape and magnetization of a single MNG are affected by the distribution of crosslinkers: uniform, with a displaced centre of mass, with Gaussian distribution from the centre to the periphery and reverse. The impact of a topology in a combination with an external magnetic field on MNG's viscoelastic and magnetic characteristics of the suspensions is also explored.

CPP 3.4 Mon 10:15 ZEU 255

Incorporation of Hydrophilic Microgels at Water in Oil Emulsion stabilized by Hydrophobic Nanospheres — •Sebastian Stock, Carina Schneider, Luca Mirau, Franziska Braun, and Regine von Klitzing — TU Darmstadt, Darmstadt, Germany

For particle-stabilized emulsions (Pickering emulsions, PEs), the affinity of the particular stabilizers to one or the other liquid decides about the resulting emulsion type - either oil in water (o/w) or water in oil (w/o). Besides specific exceptions, hydrophilic microgel particles (MGs) are only able to stabilize o/w emulsions. However, the w/o emulsion type is preferable in a multitude of applications ranging from the food industry over medicine towards interfacial catalysis. We solved this problem by using well-characterized, hydrophobic, positively charged, spherical silica particles (SNs) and hydrophilic, positively charged PNIPAM MGs to stabilize water in 1-dodecene emulsions simultaneously. Using these thoroughly characterized model particles allows deep insights into the interplay between soft and solid particles at the interface and the structure formation of the PEs. The interaction between different kinds of particles was studied on a Langmuir trough in combination with AFM measurements. The observable structure formation at the interface of the Langmuir Trough could explain the particle assembly at the droplet interfaces in PEs.

CPP 4: Active Matter I (joint session BP/CPP/DY)

Time: Monday 9:30–13:00 Location: TOE 317

Invited Talk CPP 4.1 Mon 9:30 TOE 317

Emergent properties in motile active matter — •Roland G. Winkler — Theoretical Physics of Living Matter (IBI-5/IAS-2), Forschungszentrum Jülich, Jülich

Motile active matter systems, ranging from assemblies of bacteria, self-organized bio-polymers such as the cytoskeleton of living cells, to schools of fish and flocks of birds, exhibit intriguing emerging structural and dynamical out-of-equilibrium properties, even with reminiscence to classical turbulence. Their spatiotemporal dynamics is controlled by the propulsion of the active agents in combination with various direct interactions. The latter are typically anisotropic and emerge from different sources, such as elongated agent shapes, intrinsic flexibility and constraints, microswimmer flow fields etc. By analytical theory and mesoscale simulations, we study the physical aspects of motile active matter, ranging from propulsion of bacteria and linear filaments to large-scale collective properties of active agents, and unravel its generic features. Studies on individual polymers reveal fundamental differences in their dynamical and conformational properties depending on their propulsion mechanism, which is illustrated for polymers either tangentially driven or composed of active Brownian particles. In the latter case, hydrodynamic interactions additionally affect the conformational properties, in contrasts to passive polymers. Moreover, hydrodynamic interactions determine the activity-induced phase behavior. For spherical microswimmers (squirmers), hydrodynamics suppresses motility-induced phase separation, but enhances collective turbulent-like large-scale flows.

CPP 4.2 Mon 10:00 TOE 317

High-resolution mapping of odd fluctuations and oscillations in living chiral crystals — •Jinghui Liu[1,2], Lisa Lin[1], Yuchao Chen[1], Yu-Chen Chao[1], and Nikta Fakhri[1] — [1]Department of Physics, Massachusetts Institute of Technology — [2]Center for Systems Biology Dresden

It has been shown that active crystals formed by self-assembling clusters of swimming starfish embryos exhibit signatures of odd mechanics, such as self-sustained chiral waves. How are these observed chiral waves and oscillations are actuated and how their dynamics couple to the formation and dissolution of the living chiral crystal? Here, we report the use of vibrational mode decomposition to dissect various non-equilibrium phases of the crystal dynamics. By analyzing embryo cluster trajectories over the time course of crystal formation and dissolution, we identify the spatial modes responsible for the collective actuation of an oscillatory active crystal both in spontaneous and mechanically excited conditions. We also report a direct extraction of dispersion relation from fluctuations of confined crystals to infer odd elastic moduli. Taken together, our results unveil the complex spatiotemporal origin of mechanical waves in non-reciprocal materials and provide insight on the design principles of collective phases of active metamaterials.

CPP 4.3 Mon 10:15 TOE 317

Self-organized chemotaxis of coupled cell populations — •Mehmet Can Ucar and Edouard Hannezo — Institute of Science and Technology Austria, Am Campus 1, 3400 Klosterneuburg, Austria

Many processes in development and disease such as tissue morphogenesis, cancer invasion and immune response rely on collective directional movement of cells. In a wide array of systems this collective motility is driven locally by self-generated chemokine or stiffness gradients, as opposed to pre-patterned, global guidance cues. While recent studies have explored migration mechanisms of a single species of cells, the role of self-generated gradients navigating multiple cell types remains largely untested. Here we address this issue by introducing a theoretical framework for self-organized guidance of chemotactically coupled cell populations. Combining analytical theory and simulations with experiments on immune cell populations, we discover a diverse spectrum of collective migration patterns controlled by single-cell properties. We find that differential chemotactic sensitivity leads to efficient colocalization of distinct cell types, and show that this coupling also depends on the geometry and initial configuration of the dynamical system. We finally outline conditions for robust, sustained multicellular interactions relevant for physiological settings such as during immune response.

CPP 4.4 Mon 10:30 TOE 317

Geometry-induced patterns in collective cell migration — •David Brückner — Institute of Science and Technology, Am Campus 1, 3400 Klosterneuburg, Austria

The coordinated migration of cell collectives is increasingly well understood at the level of large two-dimensional confluent monolayers. However, many physiological migration processes rely on small polarized cell clusters and their responses to external confining geometries, such as 2D channels and 3D curved environments. How active motion and cell-cell interactions interplay with such external boundaries remains poorly understood. I will discuss how external geometries can induce patterns in collective cell migration, using two examples. First, we show that the migration efficiency of 2D confined cell clusters is determined by the contact geometry of cell-cell contacts that are either parallel or perpendicular to the direction of migration. Our minimal active matter model reveals how cell-cell interactions determine a geometry-dependent supracellular stress field that controls this response to external boundaries. Secondly, we show how the interplay of curvature and active flocking dynamics of 3D cell spheroids induces a collective mode of cell migration manifesting as a propagating velocity wave. Together, these approaches provide a conceptual framework to understand how cell-cell interactions interplay with 2D and 3D geometries to determine the emergent dynamics of collective cell migration.

CPP 4.5 Mon 10:45 TOE 317

Shape primed AC-electrophoretic microrobots — •Florian Katzmeier and Friedrich C. Simmel — Technical University of Munich, Munich, Germany

Second-order electrokinetic flow around colloidal particles caused by concentration polarization electro-osmosis can be utilized to controllably move asymmetric particle dimers in AC electrical fields. To demonstrate this actuation mechanism, we created particle dimers from micron-sized silica spheres with sizes 1.01 μm and 2.12 μm by connecting them with DNA linker molecules. The dimers can be steered along arbitrarily chosen paths within a 2D plane by controlling the direction of the AC electric field in a fluidic chamber with the joystick of a gamepad. Further utilizing induced dipole-dipole interactions, we demonstrate that particle dimers can be used to controllably pick up monomeric particles and release them at any desired position, and also to assemble several particles into groups. Systematic experiments exploring the dependence of the movement direction and velocity on buffer composition, frequency, and field strength further elucidate the underlying physical mechanism, and provide operational parameter ranges for our micro robotic swimmers which we termed 'SPACE-bots'.

15 min. break

CPP 4.6 Mon 11:15 TOE 317

Rodrolls: self-rolling rods powered by light and chemical gradients — •Ann Rosna George[1], Martin Wittmann[2], Antonio Stocco[1], Igor M. Kulić[1], and Juliane Simmchen[2] — [1]CNRS, Institute Charles Sadron, Strasbourg, France — [2]Physical chemistry, TU Dresden, Germany

The self-rolling motion upon spontaneous symmetry breaking is demonstrated by certain rod-shaped microorganisms like viruses. Hence it is imperative that we understand the mechanism of this symmetry breaking triggering the active rolling motion. This behaviour has also been demonstrated on the macroscopic scale by rod-like objects. It is very interesting to try and replicate this on a microscopic scale. The main aim of the project is to create a new class of active rods that exhibit rolling activity under chemical and optical gradients. To achieve this, it is important to understand the mechanism of activity of rod-like objects under chemical and optical stimuli.

Experiments conducted using silica Janus rods with a Platinum layer in an aqueous solution of H2O2 give interesting results and exhibit different kinds of activity when parameters like concentration of H2O2 and aspect ratio of rods are changed. Under specific conditions, particles are capable of switching their direction of motion. Experiments done using rods covered in gold nanoparticles under an optical gradient also reveal promising results of being able to make the rods roll upon providing sufficient energy to break the symmetry and fine-tuning certain parameters.

CPP 4.7 Mon 11:30 TOE 317

Active Nematic Multipoles: Flow Responses and the Dynamics of Defects and Colloids — •Alexander J. H. Houston[1,2] and Gareth P. Alexander[1,3] — [1]Department of Physics, Gibbet Hill Road, University of Warwick, Coventry, CV4 7AL, United Kingdom — [2]Department of Physics, University of York, Heslington, York YO10 5DD, United Kingdom — [3]Centre for Complexity Science, Zeeman Building, University of Warwick, Coventry, CV4 7AL, United Kingdom

Two fundamental questions in active nematics are how to extract useful work from their non-equilibrium dynamics and how to extend the topological defect-based description of dynamics that has proved useful in two dimensions to three dimensions, in which the defects form geometrically-complex loops. We introduce a general description of localised distortions in active nematics using the framework of 'active nematic multipoles'. We give the Stokesian flows for arbitrary multipoles in terms of differentiation of a fundamental flow response and describe them explicitly up to quadrupole order. This allows the identification of the dipolar and quadrupolar distortions that generate self-propulsion and self-rotation respectively and serves as a guide for the design of arbitrary flow responses. Our results can be applied to both defect loops in three-dimensional active nematics and to systems with colloidal inclusions. They reveal the geometry-dependence of the self-dynamics of defect loops and provide insights into how colloids might be designed to achieve propulsive or rotational dynamics, and more generally for the extraction of work from active nematics.

CPP 4.8 Mon 11:45 TOE 317

Structure and Dynamics of Active Polymer — •Sunil Pratap Singh — Indian Institute of Science Education and Research Bhopal, India, 462066

In this talk we are going to present structural and dynamical properties of a self-propelled filament using coarse-grained Brownian dynamics simulations. We consider two kinds of self-propulsion force on polymers, in case one force is applied tangent to the filament and in another model direction of active force is considered to be random. Case one shows that chain's stiffness and radius of gyration monotonically decrease. Moreover, the radius of gyration of the filament shows universal scaling for various bending rigidities with flexure number. In the latter model, where monomers are assumed to be active Brownian particle (ABP), displays a non-monotonic behaviour of end-to-end distance with activity strength. We will discuss here the role of many-body interactions on its structure and relaxation behavior. Additional we talk about the rheological behavior of chain under linear shear-flow. Our simulations reveal that active polymer's zero-shear viscosity varies in non-monotonic fashion with the active noise. More-importantly the viscosity decreases in the intermediate regime, that is followed by an increase in the more extensive Pe regime. We attribute the decrease of the zero-shear viscosity in the intermediate regime is due to many-body interactions among chain monomers.

CPP 4.9 Mon 12:00 TOE 317

Pumping, Mixing, and Signal Transmission in Active Pores — •Goncalo Antunes[1,2,3], Paolo Malgaretti[1,2,3], Siegfried Dietrich[2,3], and Jens Harting[1,4] — [1]Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien (IEK–11), Forschungszentrum Jülich, Cauer Str. 1, 91058 Erlangen, Germany — [2]Max–Planck–Institut für Intelligente Systeme, Heisenbergstr. 3, 70569 Stuttgart, ,Germany — [3]IV. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [4]Department Chemie- und Bioingenieurwesen und Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Fürther Straße 248, 90429 Nürnberg, Germany

Much attention is currently being given to the problem of manipulating fluids at the microscale, with successful applications to fields such as 3D fabrication and biomedical research. An intriguing technique to manipulate fluid flows in a pore is diffusioosmosis. We show both numerically and analytically that a corrugated catalytic pore can act as a micropump even when it is fore-aft symmetric. This phenomenology is possible due to a spontaneous symmetry breaking which occurs when advection rather than diffusion is the dominant mechanism of solute transport. Relaxing the condition of Stokes flow leads to unsteady flow, and persistent oscillations with a tunable frequency appear. We further include the inverse chemical reaction that consumes solute and introduces an additional timescale. Finally, we find that the flow may lose its axial symmetry and hence promote mixing in the low Reynolds number regime.

CPP 4.10 Mon 12:15 TOE 317

Interacting particles in an activity landscape — •Adam Wysocki[1], Anil Kumar Dasanna[1,2], and Heiko Rieger[1,2] — [1]Department of Theoretical Physics and Center for Biophysics, Saarland University, Saarbrücken, Germany — [2]INM-Leibniz Institute for New Materials, Saarbrücken, Germany

We study interacting active Brownian particles (ABPs) with a space-dependent swim velocity. We find that, although an equation of state exists, a mechanical equilibrium does not apply to ABPs in activity landscapes. The pressure imbalance originates in the flux of polar order across the interface between regions of different activity. An active-passive patch system is mainly controlled by the smallest global density for which the passive patch can be close packed. Below this density a critical point does not exist and the system splits continuously into a dense passive and a dilute active phase with increasing activity. Above this density and for sufficiently high activity the active phase may start to phase separate into a gas and a liquid phase caused by the same mechanism as motility-induced phase separation of ABPs with a homogeneous swim velocity.

CPP 4.11 Mon 12:30 TOE 317

Active phase fluctuations of Chlamydomonas axonemes — •Abhimanyu Sharma[1], Benjamin M. Friedrich[2], and Veikko F. Geyer[1] — [1]B CUBE - Center for Molecular Bioengineering, TU Dresden, Dresden, Germany — [2]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany

Cilia and eukaryotic flagella generate periodic beat patterns by the activity of dynein motors. Earlier studies revealed active fluctuations in the ciliary beat arising presumably from small number fluctuations in the collective dynamics of the molecular motors that drive the beat. A theoretical model of the beating cilium as a system of coupled motors predicts that the fluctuations measured in terms of the quality factor of the oscillations scale with the number of beat-generating-motors.

To measure those fluctuations experimentally, we use in situ reactivated axonemes, the mechanical core of motile cilia isolated from the green alga Chlamydomonas. To modulate the number of motors in beating axonemes, we make use of motor mutants or partially extract molecular motors biochemically.

Using shape mode analysis and limit-cycle reconstruction, we characterize the phase fluctuations in the beat and report for the first time the relation between beat parameters and the motor number in Chlamydomonas axonemes. We experimentally infer scaling relations for the beat frequency, mean beat amplitude, and the quality factor. Further, using mass spectrometry, we identify specific dynein motors and infer their role in regulating the beat fluctuations.

CPP 4.12 Mon 12:45 TOE 317

Lattice dynamics of pulsating active particles — •Alessandro Manacorda and Étienne Fodor — University of Luxembourg

Cells in epithelial tissues can drastically deform their shapes and volume giving rise to collective behavior such as size oscillation and wave propagation. These phenomena have a strinking impact in many biological contexts such as embryonic development, cardiac arrhythmias and uterine contraction.

The theoretical models describing the emergence of contractile waves so far consider the cells as motile particles, where activity is represented by self-propulsion; however this ingredient is questionable in dense systems where particles barely move. We therefore introduce a novel class of active matter where the activity is the ability to change an internal degree of freedom at the single-particle level e.g. particles' size. The collective behavior of active particles is investigated in a lattice model, where the interplay between pulsation and synchronization gives rise to emergent behavior such as wave propagation. Fluctuating hydrodynamic equations can be obtained from microscopic dynamics and their predictive power is shown in comparison with numerical simulations.

We highlight the minimal ingredients needed for the complex behavior above-mentioned and point out future directions in the growing field of pulsating active matter.

CPP 5: 2D Materials I (joint session HL/CPP)

Time: Monday 9:30–12:30 Location: POT 81

CPP 5.1 Mon 9:30 POT 81

Spin-valley physics in strained transition metal dichalcogenides monolayers — •Paulo E. Faria Junior[1], Klaus Zollner[1], Tomasz Woźniak[2], Marcin Kurpas[3], Martin Gmitra[4], and Jaroslav Fabian[1] — [1]University of Regensburg, Regensburg, Germany — [2]Wroclaw University of Science and Technology, Wroclaw, Poland — [3]University of Silesia, Chorzów, Poland — [4]Pavol Jozef Šafárik University in Košice, Košice, Slovakia

Transition metal dichalcogenides (TMDCs) are ideal candidates to explore the manifestation of spin-valley physics under external stimuli. Here, we investigate the influence of strain on the spin, orbital angular momenta and g-factors of monolayer TMDCs within first principles[1]. Our calculations reveal the behavior of direct exciton g-factors under the isolated impact of strain: tensile (compressive) strain increases (decreases) the absolute value of g-factors. Strain variations of 1% modify the bright (A and B) exciton g-factors by 0.3 (0.2) for W (Mo) based compounds and the dark exciton g-factors by 0.5 (0.3) for W (Mo) compounds, suggesting that strain can be responsible for g-factor fluctuations observed experimentally. We complete our analysis for the Gamma and Q valleys, revealing that the spin degree of freedom dominates. This fundamental microscopic insight into the role of strain in the spin-valley physics of TMDCs is crucial to understand recent experiments[2,3]. [1] Faria Junior et al., NJP 24, 083004 (2022). [2] Covre, Faria Junior et al., Nanoscale 14, 5758 (2022). [3] Blundo, Faria Junior et al., PRL 129, 067402 (2022). Funding: DFG SFB 1277, SPP 2244.

CPP 5.2 Mon 9:45 POT 81

A bright single-photon source based on a WSe$_2$ monolayer in an open cavity — •Victor Mitryakhin[1], Hangyong Shan[1], Jens-Christian Drawer[1], Sven Stephan[1], Martin Silies[2], Falk Eilenberger[3], Carlos Antón-Solanas[1], Martin Esmann[1], and Christian Schneider[1] — [1]Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg, Germany — [2]Hochschule Emden/Leer, 26723 Emden, Germany — [3]Friedrich-Schiller-Universität Jena, 07745 Jena, Germany

Single photon sources based on crystalline defects present in transition-metal dichalcogenide monolayers, 2D atomically thin direct-bandgap semiconductors, have recently emerged as a promising platform for realization of and use in quantum communication and information processing.

In this work, we investigate the properties of single photon emission from a single exciton in a WSe$_2$ monolayer weakly coupled to an asymmetric plano-concave microcavity consisting of freely movable mirrors in 3 directions. In this regard, it enables us for an in-situ control of the properties of the emission and the extraction efficiency of single photons in the device.

We report a highly bright and linearly polarized single photon source with source brightness exceeding 70 % under saturation conditions, polarization degree of 98.4 ± 1.3 % and high photon purity noted by the second-order correlation $g^{(2)}(0)$ value of 0.047 ± 0.007, measured in Hanbury-Brown-Twist type of a setup.

CPP 5.3 Mon 10:00 POT 81

Strong coupling of excitons in a WS2-monolayer coupled to a silver nanogroove array — •Yuhao Zhang[1], Hans-Joachim Schill[1,2], Stephan Irsen[2], and Stefan Linden[1] — [1]Physikalisches Institut, Universität Bonn — [2]Center of Advanced European Studies and Research (caesar)

In this work, we report on room-temperature interaction of a WS2 monolayer with a tapered nanogroove array milled into monocrystalline silver flake. The bare nanogroove array features three polariton branches resulting from the coupling of localized surface plasmon modes (LSPR) in the nanogrooves and propagation surface plasmon modes (SPP). The linewidth of the lower plasmon polariton branch critically depends on the geometry of the nanogrooves. When a WS2 monolayer is deposited on the nanogroove array with optimized damping, the reflection spectra show an avoided crossing of the exciton mode and the lower plasmon polariton branch with a Rabi splitting of 38.7 meV indicating strong exciton-plasmon polariton coupling.

CPP 5.4 Mon 10:15 POT 81

Theory of exciton localization in TMDCs using metal nanoparticles — •Robert Salzwedel[1], Lara Greten[1], Stefan Schmidt[1], Chelsea Carlson[2], Stephen Hughes[2], Malte Selig[1], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany — [2]Department of Physics, Queen's University, Kingston, Ontario, Canada

In recent years, monolayers of transition metal dichalcogenides (TMDCs) have attracted considerable attention due to their strong Coulomb and light-matter interactions, leading to tightly bound excitons with large optical oscillator strength. Due to the finite thickness of the monolayers, these excitons are very sensitive to the environment, which allows their properties to be tailored, e.g., by functionalization with molecules or metal nanoparticles (MNPs) [1,2].

We present a theory based on a self-consistent solution of Maxwell's and Bloch equations to analytically study a coupled system of MNP plasmons and TMDC excitons. For the combined system, we identify an effective eigenvalue equation that governs the center of mass motion of the dressed excitons in a plasmon-induced potential. Examination of the ensuing plexcitonic equation reveals the existence of bound states, which we interpret as excitons localized in the external potential. The appearance of these bound states in this potential is an indicator of strong coupling between excitons and plasmons.

[1] Carlson et al. (2021). PRB, 104(12), 125424.
[2] Denning et al. (2022). PRB, 105(8), 085306.

15 min. break

CPP 5.5 Mon 10:45 POT 81

Electronic effects of non-uniformly strained 2D TMDCs — •Mohammadreza Daqiqshirazi and Thomas Brumme — Chair of Theoretical Chemistry, Technische Universität Dresden, Bergstraße 66c, 01069 Dresden, Germany

Strain plays an important role in most 2D materials since there is a strong influence of the strain state on the relative band alignment of different valleys in the electronic band structure. The effects of non-uniform strain on the properties of 2D materials are scarcely studied theoretically, even if in experiments a lot of different structures can be found in which a spatial varying strain state is present such as wrinkles or folds. Here, we are investigating how such non-uniform strain influences the electronic properties of the prototypical 2D materials WSe2 and MoS2.We study nanoscale wrinkles and nanotubes in detail and discuss important differences in the strain distribution and magnitude, also to understand if nanotubes could be used as a model system for non-uniformly strained systems. Using Density Functional Theory we find that the inclusion of spin-orbit interaction is crucial to correctly predict the changes in the band structure of wrinkled 2D materials as the non-uniform strain changes the symmetry compared to a flat layer. This introduces a strong Rashba-like splitting of the valence-band maximum near the Γ point. The situation complicates even more with the addition of an extra layer forming a bilayer or a hetrobilayer. The spatial varying band alignments in wrinkled multilayers can lead to new interlayer excitons which are confined to certain regions of the system.

CPP 5.6 Mon 11:00 POT 81

Optical properties of monolayer ReSe$_2$ and ReS$_2$ — •Thorsten Deilmann — Institute of Solid State Theory, University of Münster, Germany

Rhenium-based transition metal dichalcogenides unite the fascinating characteristics of the confined in-plane physics with their reduced crystal symmetry. This paves the way for polarization-sensitive applications, such as optical logic circuits operating in the infrared spectral region.

Here, we investigate the doping-dependent optical properties of ReSe$_2$ and ReS$_2$ from first principles. Besides strong excitonic effects, recent experimental studies have reported three-particle states (i.e. trions) with trion binding energies of more than 100 meV [1,2]. Using our ab initio methods we are able to predict neutral and charged properties and find much smaller binding energies compared to experiment.

[1] Advanced Functional Materials, 10, 1905961 (2019)
[2] Applied Physics Letters 119, 113103 (2021)

CPP 5.7 Mon 11:15 POT 81

Evaluating Atomically Thin Single-Photon Sources for Quantum Key Distribution — •Timm Gao[1], Martin v. Helversen[1], Carlos Anton-Solanas[2], Christian Schneider[2], and Tobias Heindel[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

Quantum light sources are considered key building blocks for future quantum communication networks. In recent years, atomic monolayers of transition metal dichalcogenides (TMDCs) emerged as a promising material platform for the development of compact quantum light sources. In this work, we evaluate for the first time the performance of a single-photon source (SPS) based on a strain engineered WSe_2 monolayer [1] for applications in quantum key distribution (QKD) [2]. Employed in a QKD-testbed emulating the BB84 protocol, an antibunching of $g^{(2)}(0) = 0.127 \pm 0.001$ and a raw key rate of up to (66.95 ± 0.10)kHz make this source competitive with previous SPS based QKD experiments using quantum dot based SPSs. Furthermore, we exploit routines for the performance optimization previously applied to quantum dot based single-photon sources [2]. Our work represents an important step towards the application of TMDC-based devices in quantum technologies.

[1] L. Tripathi et al., ACS Photonics 5, 1919-1926 (2018)
[2] T. Gao et al., arXiv:2204.06427 (2022)
[3] T. Kupko et al., npj Quantum Information 6, 29 (2020)

CPP 5.8 Mon 11:30 POT 81

Theory of Thermalization of Excitons at Elevated Densities in Atomically Thin Semiconductors — •Manuel Katzer, Andreas Knorr, and Malte Selig — Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Atomically thin semiconductors exhibit tightly bound electron-hole pairs which stimulated exciton research in recent years [1]. So far, many studies focused on the understanding of exciton dynamics in the limit of very dilute systems. Recent experimental findings [2] raised the question of the excitonic thermalization behaviour for densities above this dilute, classical limit. Due to the co-bosonic nature of excitons [3], we find both bosonic but also fermionic contributions to the thermalization, with the fermionic Pauli blocking effects being dominant for a broad range of parameters. Based on a Heisenberg equation of motion ansatz [4], we discuss the first order of non-linear exciton-phonon interaction exceeding the classical Boltzmann scattering limit, in order to analyze the character of the exciton thermalization at elevated excitation densities.
[1] Wang et al. RMP 90, 021001 (2018). [2] Sigl et al. PRR 2 (4), 042044 (2020). [3] Katsch et al., PRL 124 25 257402 (2020). [4] Selig et al. PRR, 1, 022007 (2019).

15 min. break

CPP 5.9 Mon 12:00 POT 81

Strong exciton-plasmon coupling in hybrids of 2D semiconductors and plasmonic crystals — •Lara Greten[1], Robert Salzwedel[1], Stephen Hughes[2], Malte Selig[1], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany — [2]Department of Physics, Queen's University, Kingston, Canada

Monolayers of transition metal dichalcogenides (TMDCs) are direct-gap semiconductors that exhibit tightly bound excitons with pronounced optical amplitudes. Thus, they are promising for various optoelectronic applications and an excellent material to investigate excitons. Another material with a large optical amplitude is a plasmonic crystal - arrays of metal nanoparticles - which supports collective plasmon modes, and yields amplification of the electric fields on the nanoscale.

Here, we theoretically consider exciton-plasmon coupling in a hybrid structure of a TMDC layer interacting with a plasmonic crystal with a 2d lattice. Our study reveals a hybridization of plasmons and initially momentum dark excitons. In addition, we find an excitonic mode with negligible coupling to the plasmonic near field, emitting undisturbed radiation into the far field. To connect to related experiments, we compute the scattered light in the near- and far-field explicitly and identify signatures of strong exciton-plasmon coupling with a Rabi splitting of more than 100 meV. We also find that the uncoupled exciton mode results in a third peak at the undisturbed exciton energy.

CPP 5.10 Mon 12:15 POT 81

Enhancement of Light Emission in Hexagonal Boron Nitride Structures — •Felix Schaumburg, Marcel Zöllner, Vasilis Dergianlis, Stephan Sleziona, Marika Schleberger, Axel Lorke, Martin Geller, and Günther Prinz — Faculty of Physics and CENIDE, University Duisburg-Essen, Germany

Optical spectroscopy, especially Raman- and photoluminescence (PL)-spectroscopy, is commonly used to study the optical properties of 2D materials. In order to obtain the highest Raman/PL-signals, it is important to reduce the reflection of the excitation laser.

We studied a number of exfoliated hexagonal Boron Nitride (hBN) flakes with different thicknesses on a Si substrate with a 300 nm SiO_2 top layer. By changing the hBN layer thickness, we found a specific thickness, where all Raman signals (from Si, SiO_2 and hBN) showed maximum intensity, whereas the backscattered laser light was suppressed. To explain the increased intensities, we calculated the reflectivity and transmissivity of the full layer system (air, hBN, SiO_2, Si) for different hBN layer thicknesses and for different excitation wavelengths (457 nm, 532 nm, 633 nm), using the transfer-matrix-algorithm. To compare theory with experiment, we performed Raman measurements with the 3 different wavelengths on different flakes and determined their thicknesses with AFM-measurements.

Our results are in good agreement with theory and show that it is possible to choose the best flakes for spectroscopy, just by looking at their color in an optical microscope. This also allows us to easily find good flakes for observation of efficient single defect emission.

CPP 6: Perovskite and photovoltaics I (joint session HL/CPP)

Time: Monday 9:30–12:30 Location: POT 251

CPP 6.1 Mon 9:30 POT 251

Bandgap engineering of two-step processed perovskite top cells for application in perovskite-based tandem photovoltaics — •Ronja Pappenberger[1,2], Alexander Diercks[2], Ahmed Farag[1,2], Paul Fassl[1,2], and Ulrich W. Paetzold[1,2] — [1]Institut für Mikrostrukturtechnologie, KIT, Germany — [2]Lichttechnisches Institut, KIT, Germany

Tandem solar cells offer a promising concept of raising the efficiency of silicon solar cells above the theoretical limit of 29%. In this context, silicon is supplemented by a wide-bandgap perovskite top solar cell to make better use of the solar spectrum. Perovskite solar cells come into play given their favorable optoelectronic quality and tunable bandgap. Textured-front perovskite silicon tandem solar cells currently promise the highest energy yield for modules in the field. To avoid shunting, ensure high efficiency and economic production of the perovskite on the μm-sized pyramids, a conformal growth of the perovskite layer as well as a sufficient layer thickness are necessary. A two-step method - containing a separate deposition of the PbI_2 and the organic cations - enables high film quality, flexibility in choice of component/solution and the possibility of upscaling. Here, we investigate different strategies of increasing the bandgap of the perovskite. Thereby the location of the added bromine - cation solution and/or PbI_2 solution - is critical. With our approach, the device performance - PCE of 17.2%, FF of 76% and V_{oc} of 1.156 V ($E_g \approx 1.64$ eV) - and film quality can be maintained. Furthermore, the effect of an increasing bandgap in combination with planar/textured silicon bottom cells is studied.

CPP 6.2 Mon 9:45 POT 251

Application of plasma enhanced atomic layer deposition process of alumina on perovskite film boosts efficiency of solar cells — •Małgorzata Kot[1], Mayank Kedia[2], Paul Plate[3], Ludwig Marth[3], Karsten Henkel[1], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Konrad-Zuse-Strasse 1, 03046 Cottbus, Germany — [2]Institut fuer Photovoltaik Universitaet Stuttgart, Pfaffenwaldring 47, 70569 Stuttgart, Germany — [3]SENTECH Instruments GmbH, Schwarzschildstraße 2, 12489 Berlin, Germany

It is assumed that plasma-enhanced atomic layer deposition (PEALD) cannot be used to prepare thin films on sensitive organic-inorganic perovskites because the plasma destroys the perovskite film and thus deteriorates its photophysical properties. Here, we prove that using an appropriate geometry of the ALD system (SENTECH SI PEALD system) and suitable process parameters it is possible to coat perovskites with alumina by PEALD. Spectromicroscopy followed by electrical characterisation reveal that as long as the PEALD process is not optimized (too long plasma pulses) one gets degradation of the perovskite as well as dissociation of the created iodine pentoxide (during PEALD) under light that causes a valence band maximum (VBM) shift to the Fermi level and thus significantly decreases the solar cell efficiency. However, once the PEALD process parameters are optimized, no VBM shift is observed. Moreover, the solar cell efficiency depends inversely on process temperature and layer thickness.

CPP 6.3 Mon 10:00 POT 251

Tuning Crystallization for Highly Efficient Perovskite Silicon Tandem Solar Cells — •Mohamed Mahmoud[1,2], Oussama Er-Raji[1,2], Patricia Schulze[1], Anna Juliane Borchert[1,2], and Andreas W. Bett[1,2] — [1]Fraunhofer ISE — [2]University of Freiburg

Perovskite solar cells have the advantages of a strong absorption edge, defect tolerance, and potential cheap production due to easy production methods such as spin coating or slot-die coating as a highly scalable production method. In the industry, double-sided textured (micro-meter sized pyramid) silicon is commonly produced to decrease reflection losses and improve light trapping. Solution-based processing methods of perovskite on top of the textured Si showed low conformality, which resulted in shunts and non-working solar cells. To overcome this issue, the hybrid route was developed, in which inorganic precursors are co-evaporated using the thermal vapor deposition technique and then organic precursors are spin-coated followed by a thermal annealing. By doing that, high conformality of perovskite thin films on top of the textured silicon is achieved. However, the resulting perovskite grain size is rather low, which can lower the bulk quality. In this work, various additives were used to increase the grain size, and their working mechanisms were studied. In addition, we study the consequences of different grain sizes at the tandem level with respect to device efficiency as well as stability. Moreover, using the thermodynamics fundamentals of crystallization, we hypothesize for the first time a common general explanation for the working mechanism of all the different additives used.

CPP 6.4 Mon 10:15 POT 251

Efficient Modeling Workflow for Accurate Electronic Structures of Hybrid Perovskites — Julian Gebhardt[1,2], •Wei Wei[1,2], and Christian Elsässer[1,2,3] — [1]Fraunhofer IWM, 79108 Freiburg — [2]Cluster of Excellence livMatS, University of Freiburg — [3]Freiburg Materials Research Center, University of Freiburg

Hybrid organic-inorganic halide perovskites are the most promising photovoltaic absorber materials to substitute or complement silicon in high-efficiency solar cells. These hybrid materials are often constrained by their low stability and critical elements like lead. Computational high-throughput screening studies, based on solid-state electronic-structure theory, are useful to identify promising substitute materials with targeted properties. In this work, we present an efficient computational approach based on density-functional theory, which is suitable to predict band gaps for arbitrary compounds reliably and in good quantitative agreement with experimental band gap data for known compounds. This approach is described and demonstrated for the building blocks of one of the most promising hybrid perovskites, namely, $(HC(NH_2)_2)_xCs_{1-x}Pb(I_yBr_{1-y})_3$, with x and y varied between zero and one.

J. G. et al. *J. Phys. Chem. C* **2021** 125, 18597.

CPP 6.5 Mon 10:30 POT 251

Photon Management for Ultrathin Solar Cells: Enabling Waveguide Modes by Structured Back Contact — •Merve Demir, Thomas Schneider, Torsten Hölscher, Heiko Kempa, and Roland Scheer — Martin-Luther-Universität Halle-Wittenberg, Germany

The recent research based on Cu(In,Ga)Se2 (CIGSe) solar cells is focused on thinning down the absorber layer to enable less material consumption and cost effective large scale production. However, having ultra-thin CIGSe solar cells with absorber layer thickness in sub-micron level brings the cost of limited absorption of solar spectra and hence leads to lower energy conversion efficiencies. This problem can be overcome by the cell architecture including functional back contact elements for the enhancement of optical absorption. In this contribution, ultrathin CIGSe solar cells with 500 nm thick absorber layer were combined with nano-textured SiO2 back contacts together with aluminum back mirror. With this cell design, it is aimed to have increased power conversion efficiency for ultra-thin CIGSe solar cells due to enhanced absorption of long wavelength region photons. The solar cell parameters were extracted and compared with the conventional CIGSe back contact, flat molybdenum, to reveal the effects of functional back contact. The experimental findings on quantum efficiency measurements prove the positive effects of having highly reflective and textured back contact. Furthermore, the growth of CIGSe on textured substrates was examined throughout cross section cuts by scanning electron microscopy and energy dispersive X-ray diffraction.

30 min. break

CPP 6.6 Mon 11:15 POT 251

Employing three-dimension structure analysis: digital twin for studying grain boundary effects in thin film solar cells — •Chang-Yun Song[1], Matthias Maiberg[1], Heiko Kempa[1], Ali Gholinia[2], Wolfram Witte[3], Dimitrios Hariskos[3], Daniel Abou-ras[4], and Roland Scheer[1] — [1]Martin-Luther-University Halle-Wittenberg, Halle, D — [2]University of Manchester, Manchester, UK — [3]Zentrum für Sonnenenergie- und Wasserstoff-Forschung, Stuttgart, D — [4]Helmholtz-Zentrum Berlin, Berlin, D

Grain boundaries (GBs) in polycrystalline Cu(In,Ga)Se2 (CIGSe), are believed to be one of the performance limiting factors of current record efficiency CIGSe solar cells. Numerous simulation studies have been conducted to unveil their effects. Most simulations, however, have been done within two-dimensions (2D), thereby presumably using the simplified GBs shapes. In this study, we thus present a realistic three-dimensional (3D) GB model for a high-efficiency CIGSe layer. To this end, a combination of electron backscatter diffraction and focused ion beam was applied to obtain 3D data of the CIGSe layer, which then allowed the reconstruction of the 3D grain structure into a computer model. By using the computer model as input for 3D opto-electronic simulations, we study the electronic effects of GBs on the high-efficiency solar cell under investigation bulk parameter values for the simulations were obtained through a combination of simulation and experiments, such that the solar cell is consistently described. As an outcome, the 3D simulations confirm that the effect of GB was indeed underestimated in earlier conventional 2D simulations.

CPP 6.7 Mon 11:30 POT 251

Interface Engineering to reduce non-radiative recombination losses at the perovskite/C60 interface in monolithic perovskite silicon tandem solar cells — •Johanna Modes, Patricia S. C. Schulze, Kaitlyn Mc Mullin, Maryamsadat Heydarian, Christoph Messmer, Juliane Borchert, and Andreas Bett — Fraunhofer ISE

Metal halide perovskites have emerged in recent years as a promising absorber material for solar cells with the potential to combine high power conversion efficiency with low production costs. However, significant non-radiative charge carrier recombination occurs at the perovskite interface to the contacts, thus preventing the full potential of the solar cell from being exploited. Photoluminescence quantum yield measurements clearly show that the Quasi-Fermi level splitting is reduced by evaporation of the electron contact C60 onto perovskites, leading to limited open-circuit voltage in devices. In recent literature, as well as in our investigations, different passivation layers are deposited between perovskite and the electron contact to reduce non-radiative recombination and to improve the open-circuit voltage. This is on the one hand pursued by increasing the selectivity at the contacts through field effects and band alignment and secondly by reducing defects at the interface through chemical passivation.

CPP 6.8 Mon 11:45 POT 251

Spontaneous Polarization in $\mathbf{NaNbO_3}$ — •Kisung Kang[1], Saud Bin Anooz[2], Jutta Schwarzkopf[2], Matthias Scheffler[1], and Christian Carbogno[1] — [1]The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin — [2]Leibniz-Institut fur Kristallzüchtung (IKZ)

The perovskite $NaNbO_3$ is regarded as a promising lead-free piezoelectric material, also because its polarization properties can be further tailored via strain engineering. [1] In thin films, lattice strain can be incorporated by the heteroepitaxial growth on lattice mismatch. By tuning the epitaxial strain in the films, different polymorphs with distinctively different polarization strength and orientation can be realized [2, 3]. We investigate this question by using density-functional theory at the semi-local level of theory, which we carefully validate with hybrid-functional calculations. By this means, we compute the spontaneous polarization for ten phases of $NaNbO_3$ as a function of stress and strain. In line with experiments, we confirm that the monoclinic *Pm* phase features a non-vanishing in-plane polarization, the orientation of which is independent of the strain. Conversely, the polarization direction of the orthorhombic $Pmc2_1$ phase depends on the applied tensile strain. We analyze the underlying electronic and atomistic mechanism and discuss how the relevant properties are influenced by phase transformations.

[1] N. Bein, *et al.*, *Phys. Rev. Mater.* **6**, 084404 (2022).
[2] J. Schwarzkopf, *et al.*, *J. Appl. Cryst.* **45**, 1015 (2012).
[3] S. B. Anooz, *et al.*, *Appl. Phys. Lett.* **120**, 202901 (2022).

CPP 6.9 Mon 12:00 POT 251

Peculiar bond length dependence and its impact on the band gap bowing in (Ag,Cu)(In,Ga)$\mathbf{Se_2}$ thin film alloys — •Hans H. Falk[1], Stefanie Eckner[1], Konrad Ritter[1], Sergiu Levcenko[1], Timo Pfeiffelmann[1], Edmund Welter[2], Jes Larsen[3], William N. Shafarman[4], and Claudia S. Schnohr[1] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Germany — [3]Department of Materials Science and Engineering, Uppsala University, Sweden — [4]Department of Materials Science and Engineering, University of Delaware, USA

Incorporation of Ag into Cu(In,Ga)Se_2 thin film solar cells improves several of their properties. However, with increasing Ag content, the band gap of (Ag,Cu)GaSe_2 increases even though the lattice expands and the Ga-Se bond length is predicted to decrease. This is counter-intuitive, since in other chalcopyrite alloys all bond lengths increase and the band gap decreases as the lattice expands. Therefore, we studied the element-specific average bond lengths of (Ag,Cu)GaSe_2, (Ag,Cu)InSe_2 and Ag(In,Ga)Se_2 using X-ray absorption spectroscopy for thin films grown on Mo-coated soda lime glass by a single stage co-evaporation process. As predicted, the Ga-Se bond length decreases with increasing Ag content in (Ag,Cu)GaSe_2. While the In-Se bond length of (Ag,Cu)InSe_2 shows the same behavior, Ag(In,Ga)Se_2 exhibits a dependence similar to that of Cu(In,Ga)Se_2, demonstrating that the peculiar behavior is related to mixing the group-I lattice site. Using the bond lengths we model the anion positions and estimate their effect on the band gap bowing.

CPP 6.10 Mon 12:15 POT 251

Fast diffusion of spin polarized excitons in bulk lead halide perovskites — •Sergiu Anghel[1], Dmitri R. Yakovlev[1], Dmitry N. Dirin[2], Maksym V. Kovalenko[2], Manfred Bayer[1], and Markus Betz[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, Otto-Hahn-Straße 4a, D-44227 Dortmund, Germany — [2]Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, Zürich CH-8093, Switzerland

We investigate the spin diffusion of the free "hot" excitons in FA0.9Cs0.1PbI2.8Br0.2 bulk lead halide perovskite crystal at cryogenic temperatures by employing ultrafast time- and spatial-resolved magneto-optical Kerr microscopy. We measure the spin diffusion coefficient (D_s) of the free excitons of D_s~50 cm^2/s , which is a very surprising outcome, especially in the light of the recent results obtained on bulk or two-dimensional perovskites [1,2], where D_s is at least two orders of magnitude lower. D_s shows a roughly linear dependence on pump energy whereas the dependence on pump power is much more intricate - after a certain pump power threshold we observe an anomalous, nonlinear spatial dependence of D_s. We discuss our findings in view of efficient exciton-phonon coupling and Auger processes.

[1] A. Baldwin, G. Delport, K. Leng, R. Chahbazian, K. Galkowski, K. P. Loh, and S. D. Stranks, J. Phys. Chem. Lett. 12, 4003 (2021). [2] S. D. Stranks, G. E. Eperon, G. Grancini, C. Menelaou, M. J. P. Alcocer, T. Leijtens, L. M. Herz, A. Petrozza, and H. J. Snaith, Science 342, 341 (2013).

CPP 7: Organic Semiconductors (joint session HL/CPP)

Time: Monday 9:30–11:15 Location: POT 361

CPP 7.1 Mon 9:30 POT 361

Field-induced Seebeck voltage in disordered semiconductors — •Anton Kompatscher and Martijn Kemerink — IMSEAM, University Heidelberg

For disordered semiconductors it is theorized that finite electric fields can heat up the charge carrier distribution to effective temperatures that can significantly exceed the lattice temperature. Here, we argue that this effective temperature should be able to efficiently drive a thermoelectric generator (TEG) based on the Seebeck effect.(1) Utilizing kinetic Monte-Carlo simulations we were able to show similar results when driving a TEG with temperature or field. As a model system we choose the Seebeck ratchet introduced by Büttiker, replacing temperature- with field-driven effective temperature modulation. This allowed us to compare the current predicted by theory with the simulation currents resulting in good functional agreement. Effective temperature drive offers interesting advantages. Since only the electron distribution but not the lattice itself is heated, one of the mayor loss channels in TEG, lattice thermal conductivity, can be suppressed. Additionally, there is no need for n- and p-type materials (nor for heat exchangers) and a single material is sufficient. The main issue for concrete realization lies in the very high necessary field strengths at which effective temperature becomes relevant and that somehow need to be coupled into the TEG.

1. "On the concept of an effective temperature Seebeck ratchet", Appl. Phys. Lett. 119, 023303 (2021) https://doi.org/10.1063/5.0052116

CPP 7.2 Mon 9:45 POT 361

Momentum dependent investigation of electronic excitations in β-metal-phthalocyanines — •Louis Philip Doctor and Martin Knupfer — Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Helmholtzstraße 20, 01069 Dresden

This work presents an investigation of the electronic excitations of β-metal-phthalocyanines. We prepared 120 nm thick thin films by physical vapour deposition, which afterwards underwent an annealing process. Infrared spectroscopy revealed that the annealed films were in the β-phase. The films were further characterised in the visible regime. The prominent feature in this regime is the Q-band, which consists of four peaks arising from the HOMO to LUMO transition split by solid state effects. Furthermore the dispersion of the Q-band was measured using electron energy loss spectroscopy. We found a complex momentum dependent behaviour. Most interesting is the negative dispersion of the lowest lying excitation, which also has a tremendous effect on the performance of optoelectronic devices. This redshift partially correlates with the intermolecular distance and the charge carrier transfer integrals. The latter were determined by a theoretical model, which describes the interaction of Frenkel and charge transfer excitons in metal-phthalocyanines. Our results clearly indicate a prominent influence of charge transfer excitons to the lowest electronic excitations.

CPP 7.3 Mon 10:00 POT 361

Photovoltaic and nonlinear optical properties of complex self-assembled liquid crystal structures — •Ahmad Murad[1], Alexey Eremin[1], Martin Feneberg[1], Maximilian Baumann[2], Matthias Lehmann[2], and Mohamed Alaasar[3] — [1]Otto-von-guericke-Universität, Magdeburg,Deutchland — [2]Julius- Maximilians - Universität Würzburg — [3]Martin Luther University Halle-Wittenberg, Halle (Saale),

We explore conducting and photovoltaic properties in a series of two classes of semiconducting liquid crystals. BTBT-derived polycatenary mesogens doped with fullerenes show helical network phases exhibiting a strong photovoltaic effect in a broad range of light spectrum from UV to VIS. The second class is star-shaped mesogens with subphthalocyanine core that forms self-assembled ferroelectric columnar phases. We characterise the polar order using polarisation-resolved measurements of Second Harmonic Generation (SHG). Dynamical SHG studies provide information about the switching rates and the stability of the ferroelectric states. The photovoltaic effect is demonstrated under UV exposure.

CPP 7.4 Mon 10:15 POT 361

What's special about Y6; working mechanism of Neat Y6 organic solar cell — •Elifnaz Saglamkaya[1], Artem Musiienko[2], Mohammad Saeed Shadabrooa[1], Bowen Sun[1], Sreelakshmi Chandrabose[3], Giulia Lo Gerfo M.[4], Niek F. van Hulst[4], Dieter Neher[3], and Safa Shoaee[1] — [1]University of Potsdam Disordered Semiconductor Optoelectronics Karl-Liebknecht-Strasse 24-25 14476 Potsdam-Golm — [2]Department Novel Materials and Interfaces for Photovoltaic Solar Cells, Helmholtz-Zentrum Berlin für Materialien und Energie, Kekuléstraße 5, 12489 Berlin, Germany — [3]University of Potsdam Physik und Optoelektronik weicher Materie Karl-Liebknecht-Straße 24-25 14476 Potsdam-Golm — [4]Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels, Barcelona, Spain

In this study, we analyse the working mechanism of single component small molecule acceptor Y6 solar cells with power conversion efficiencies reaching up to 4.5% and short circuit currents up to 8.4 mAcm-2.Using Hall effect, photo-Hall, and photoinduced absorption (PIA) measurements, we show that the charge photo-generation occurs in the bulk of Y6. With the aid of space charge limited current (SCLC) measurements we show that Y6 has an ambipolar charge carrier mobility. Our data shows that the limiting factor for the power conversion efficiency is fast charge recombination, which can be suppressed in presence of the transport layers, or modifying the morphology with a solvent additive.

15 min. break

CPP 7.5 Mon 10:45 POT 361

Ultrastrong light-matter coupling of J-aggregated squaraine in a room temperature open cavity — •Christoph Bennenhei[1], Lukas Lackner[1], Moritz Gittinger[1], Heiko Knopf[2], Falk Eilenberger[2], Jennifer Zablocki[3], Arne Lützen[3], Martin Silies[1], Christoph Lienau[1], Martin Esmann[1], and Christian Schneider[1] — [1]Institute of Physics, University of Oldenburg — [2]Fraunhofer-Institute for Applied Optics and Precision Engineering IOF, Jena — [3]Kekulé Institute of Organic Chemistry and Biochemistry, University of Bonn

Organic molecule exciton-polaritons in artificial lattices are an emerging platform to emulate complex electronic Hamiltonians at ambient conditions. We present J-aggregated squaraine dye (SQ) thin films [1] as a promising candidate for exciton-polaritons in optical cavities due to the high oscillator strength and tunable resonance. Using white light reflection spectroscopy, we demonstrate tunable ultrastrong coupling of light to the SQ thin film in an open cavity at room temperature [2] which we support by transfer matrix calculations. In ongoing experiments, we introduce structured photonic lattices to the open cavity to investigate the coupling of the polaritons to tailored potential landscapes. [1] M. Schulz, et al., Nat Commun 9, 2413 (2018). [2] L. Lackner, et al., Nat Commun 12, 4933 (2021).

CPP 7.6 Mon 11:00 POT 361

Room-temperature polariton lasing in anisotropic optical microcavities — •Christoph Bennenhei[1], Nils Kunte[1], Marti Struve[1], Heiko Knopf[2], Falk Eilenberger[2], Jürgen Ohmer[3], Utz Fischer[3], Martin Esmann[1], and Christian Schneider[1] — [1]Institute for Physics, Universität Oldenburg, Germany — [2]Fraunhofer-Institute for Applied Optics and Precision Engineering IOF, Jena, Germany — [3]Department of Biochemistry, Universität Würzburg, Germany

Organic molecule exciton-polaritons in artificial photonic potentials are an emerging platform to emulate electronic Hamiltonians at ambient conditions and for realizing low-threshold microlasers. In this work, we probe the polarization of polariton lasing in microcavities composed of dielectric Bragg reflectors with anisotropic indentations, enclosing the fluorescent protein mCherry. This material has been previously presented as a promising material for room-temperature polariton condensation [1,2]. Here, we experimentally show that lasing above the threshold differs distinctly for the two linearly polarized, energetically non-degenerate cavity eigenmodes. This effect leads to a drastic increase in the degree of linear polarization for the coherent photoluminescence emitted from the cavity. Our devices have relevant applications both for new types of polarized coherent light sources on chip and for accessing additional degrees of freedom in the emulation

of topological electronic lattice Hamiltonians at room temperature.
[1] S. Betzold et al. ACS Photonics 7, 384 (2020).
[2] M. Dusel et al. Nano Lett. 21, 6398 (2021).

CPP 8: Responsive and Adaptive Systems

Time: Monday 10:45–13:00 Location: ZEU 255

CPP 8.1 Mon 10:45 ZEU 255

Spreading drops of volatile oil induce long range thickness gradients in swelling hydrophobic polymer brush layers — •Özlem Kap[1], Simon Hartmann[2], Harmen Hoek[1], Igor Siretanu[1], Sissi de Beer[3], Uwe Thiele[2], and Frider Mugele[1] — [1]University of Twente, Physics of Complex Fluids, PO Box 217, 7500 AE Enschede (NL) — [2]Westfälische-Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 9, 48149 Münster (D) — [3]University of Twente, Sustainable Polymer Chem., PO Box 217, 7500 AE Enschede (NL)

Polymer brush layers are responsive materials that swell in contact with good solvents and their vapors. We combined optical experiments and numerical calculations based on gradient dynamics of a free energy density to study how fluid flow and solvent diffusion control the macroscopic spreading of (weakly) volatile oil drops and the swelling kinetics of an underlying hydrophobic polymer brush layer. The macroscopic spreading dynamics follow algebraic law with an exponent of 1/6, yet the spreading drops are found to be surrounded by halos of partially swollen polymer brushes. The width of the halos reaches values of hundreds of micrometers wide within hours to days, with thickness variations ranging from the dry thickness up to a maximum swelling ratio of ~4 close to the contact line. The halo profiles display long-living non-equilibrium steady state configurations that are controlled by the competition of two transport mechanisms, solvent diffusion through the polymer brush layer and through the vapor phase.

CPP 8.2 Mon 11:00 ZEU 255

Effect of architecture in thermoresponsive hydrogels from PEG-based tri- and tetrablock terpolymers — •Feifei Zheng[1], Wenqi Xu[1], Eirini Melampianaki[1], Anna P. Constantinou[2], Theoni K. Georgiou[2], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Technical Unversity of Munich, Garching, Germany — [2]Department of Materials, Imperial College, London, UK

Thermogels are an exciting class of stimuli-responsive materials with many promising applications ranging from the medical field to additive manufacturing. The mechanical properties in the gel state strongly depending on the architecture of the polymer [1]. Here, we address an ABC triblock terpolymer and a BABC tetrablock terpolymer consisting of the hydrophilic oligo(ethylene glycol) methyl ether methacrylate (OEGMA, A), hydrophobic *n*-butyl methacrylate (BuMA, B), and thermoresponsive di(ethylene glycol) methyl ether methacrylate (DEGMA, C). The results from dynamic light scattering on dilute solutions show that the hydrodynamic radii of the micelles formed by both, ABC and of BABC, increase strongly above 25 °C, and the solutions feature a cloud point, i.e. aggregation of the micelles sets in. By synchrotron small-angle X-ray scattering, we found that, ABC and BABC form elongated and spherical micelles, respectively. Forward scattering attributed to large aggregates is observed at temperatures above the cloud point for both terpolymers.

[1] A. P. Constantinou et al., Macromolecules, 2021, 54, 1943.

15 min. break

CPP 8.3 Mon 11:30 ZEU 255

Hydration Water Dynamics in a Thermoresponsive Polymer Solution Under Pressure — Bart-Jan Niebuur[1], Bahar Yazdanshenas[1], Feifei Zheng[1], Wiebke Lohstroh[2], Marcell Wolf[2], Marie-Sousai Appavou[3], Michaela Zamponi[3], Alfons Schulte[4], and •Christine M. Papadakis[1] — [1]Technical University of Munich, TUM School of Natural Sciences, Garching, Germany — [2]Technical University of Munich, Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [3]Jülich Centre for Neutron Science (JCNS) at MLZ, Garching, Germany — [4]University of Central Florida, Department of Physics, Orlando FL, U.S.A.

The water dynamics is key to functionality and phase behavior of synthetic and biological polymers. We investigate the dynamic behavior of hydration water in a concentrated aqueous solution of the thermoresponsive polymer poly(*N*-isopropyl acrylamide) (PNIPAM) in dependence on temperature and pressure employing quasi-elastic neutron scattering (QENS) [1]. The susceptibility spectra reveal the relaxation peak of the hydration water in addition to the known dynamic processes of bulk water. We find that the dehydration process at the phase transition depends strongly on pressure. Using perdeuterated PNIPAM along with QENS allows us to suppress the signal of the chain segments and to identify and characterize the behavior of the different types of bound water at the phase transition.

1. B.-J. Niebuur, W. Lohstroh, M.-S. Appavou, A. Schulte, C. M. Papadakis, Macromolecules 2019, 52, 1942.

CPP 8.4 Mon 11:45 ZEU 255

Topology Impact on nanoscale hydration of polymer brushes — •Apostolos Vagias[1], Andrew Nelson[2], Peixi Wang[3], Julija Reitenbach[3], Christina Geiger[3], Lucas Philipp Kreuzer[1,3], Thomas Saerbeck[4], Robert Cubitt[4], Edmondo Maria Benetti[5], and Peter Müller-Buschbaum[1,3] — [1]MLZ, TUM, Garching — [2]ANSTO, Sydney, Australia — [3]TUM School of Natural Sciences, Chair for Functional Materials, Garching — [4]ILL, Grenoble, France — [5]Polymer Surfaces Group, University of Padova, Padova, Italy

Polymer brushes have demonstrated growing interest during last years, in particular in combination with exposure to aqueous environment. By utilizing time-of-flight neutron reflectometry (ToF-NR), we correlate the swelling properties of hydrophilic cyclic grafted polymer brushes to their thermodynamics. Cyclic brushes exhibit more compact conformations with lower roughness compared to their linear analogues, due to the absence of dangling chain ends extending at the interface. In addition, due to increased interchain steric repulsions, cyclic brushes feature larger swelling ratios at the same composition and comparable molar mass. Moreover, the two topologies exhibit differences in ageing, upon repetitive swelling/drying cycles. We present a case where current Flory-like expressions breakdown in the explanation of the experimental observations.

CPP 8.5 Mon 12:00 ZEU 255

Spiropyran/Merocyanine Amphiphile in Various Solvents: A Joint Experimental-Theoretical Approach to Photophysical Properties — Vladyslav Savchenko[1], Nino Lomadze[2], Svetlana Santer[2], and •Olga Guskova[1] — [1]IPF Dresden — [2]University of Potsdam

This joint experimental-theoretical work explains the negative photochromism of spiropyran-containing (SP) amphiphile aqueous solutions. Experiments demonstrate that the orange-red merocyanine (MC) form becomes thermodynamically more stable in water, and both UV and vis stimuli lead to the partial or complete photobleaching of the solution.The explanation of this phenomenon is given on the basis of DFT calculations and MD simulations. The latter reveal that stabilization of MC in water proceeds with the energy of ca. 70 kJ/mol, and that the Helmholtz free energy of hydration of MC form is 100 kJ/mol lower. The explanation of such a difference lies in the molecular properties of the MC. The presence of three charged groups on the periphery of a flat MC backbone stimulates its self-assembly in water ending up with the formation of elongated associates with stack-like building blocks. Our quantitative evaluation of the hydrophilicity switching in SP/MC containing surfactants may prompt the search for new systems, including colloidal and polymeric ones, aiming at remote tuning of their morphology, which could give new promising shapes and patterns for the needs of modern nanotechnology. This work is supported by DFG, grant GU1510/5-1. [1] Savchenko V., et al. Int. J. Mol. Sci. 2022, 23(19), 11535

CPP 8.6 Mon 12:15 ZEU 255

Mechanochemistry: a theoretical and experimental interplay — •Michael Walter, Wafa Maftuhin, and Pooja Bhat — Albert-Ludwigs-Universität Freiburg, Freiburg i. Br., Germany

Mechanochromic polymers are intriguing materials that allow to sense force of specimens under load. The connection between macroscopic stress and the forces acting on the molecular level is still elusive and covalently incorporated molecular mechanochromophors promise to shed light on this connection. Most mechanochromic systems rely on covalent bond scission with optically distinct *on* and *off* states. Bond rupture is induced by temperature fluctuations involving force dependent barriers. We show that these barriers are fully determined by the dissociation energy and the maximal force the potential can withstand, which allows for a re-interpretation of the Eyring-Zhurkov-Bell length $\Delta x^\ddagger$ and the expressions going beyond.

We furthermore present and analyse the concept of mechanochromic donor-acceptor (DA) torsional springs that allows for a contineous mapping of molecular forces to photoluminescence wavelengths. The mechanically induced deflection from equilibrium geometry of the DA spring is theoretically predicted and reveals forces of 1 nN on the molecular level. Our theoretical analysis demonstrates a thiophene ring flip as the major part of the overall mechanochromic response within a related ansa-DAD spring at forces as low as 27 pN. Such micromechanical motion gives access to sensing of tiny forces and expands both sensitivity and the force range of conformational mechanochromophores.

CPP 8.7 Mon 12:30 ZEU 255

Humidity & Electrochemical Switching of Mixed Conducting Polymer Films — •Sabine Ludwigs — IPOC - Functional Polymers, Institute of Polymer Chemistry, University of Stuttgart

Though electrochemistry of conducting polymers is a rather old topic(1), only recently conducting polymers have received renewed attention as inherently mixed-ionic-electronic conductors for a number of emerging switchable technologies including actuators, wetting on surfaces and electrically switchable metasurfaces. One of the work-horses of the community remains poly(ethylenedioxythiophene) :poly(styrenesulfonate) (PEDOT:PSS). While typically known as synthetic metal with application as transparent flexible electrodes, the material is a mixed conductor and shows ionic conductivity which is strongly affected by humidity.(2) The humidity dependence of the PSS polyelectrolyte phase together with the electroactive nature of the PEDOT can be used to create multifunctional and multiresponsive materials and films. A recent example from my group is the preparation of intelligent humidity-triggered bilayer actuators whose bending behavior (curvature) can be explained by the humidity-dependent mechanical behavior of the constituents.(3) In collaboration with the Giessen Group the electrochemical stimuli were further used to switch nanoantennas on and off between the metallic and the insulating state.(4)

Ref: (1) Chemical Reviews 2010, 110, 4724.(2) ACS Applied Materials & Interfaces, 2020, 12, 6742. (3) Advanced Materials 2021, 202007982. (4) Science 2021, 374, 612.

CPP 8.8 Mon 12:45 ZEU 255

Stimuli-responsive high aspect ratio surfaces for wetting studies — •Gissela Constante[1], Indra Apsite[1], Paul Auerbach[2], Sebastian Aland[3], Dennis Schönfeld[3], Thorsten Pretsch[3], Pavel Milkin[1], and Leonid Ionov[1,4] — [1]Uni Bayreuth, Bayreuth, Germany — [2]HTW Dresden, Dresden, Germany — [3]Fraunhofer IAP, Postdam, Germany — [4]BPI, Bayreuth, Germany

The fabrication of switchable surfaces has been of interest in several fields such as biotechnology, industry, and others. The selection of materials and methods is crucial to provide proper control on the tunable surface. In this research, an exceptionally high aspect ratio lamellar surface topography was fabricated by melt-electrowriting of microfibers of a shape-memory thermo-responsive polyurethane. Two different types of stimuli: temperature and light exposition were applied to modify the mechanical properties and by it the deformation and recovery of the original surface. Wetting studies showed that the deformation of the high aspect ratio lamellar surface can be tunned not only manually, but as well by a liquid droplet. This behavior is controlled by variation of temperature conducted by direct heating/cooling or by exposure to light when the lamellae were stained with black ink. The liquid in combination with thermo-responsive topography presents a new type of wetting behavior. This feature opens the possibility to apply such topographies for the design of smart elements for microfluidic devices, for example, smart valves.

CPP 9: Organic Thin Films, Organic-Inorganic Interfaces (joint session DS/CPP)

Time: Monday 11:30–12:45 Location: SCH A 315

CPP 9.1 Mon 11:30 SCH A 315

Thickness dependency of the critical dose for beam-sensitive two-dimensional polymers — •David Mücke[1], Ute Kaiser[1], and Haoyuan Qi[1,2] — [1]Central Facility of Material Science Electron Microscopy, Universität Ulm, 89081 Ulm, Germany — [2]Center for Advancing Electronics Dresden (cfaed) & Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01062 Dresden, Germany

For organic materials the achievable resolution in a TEM is limited by their resilience against electron irradiation. Due to that, increasing the critical dose of these sensitive materials is of highest importance. For layer stacked materials, where the thickness is easily controllable, the thickness dependency of the critical dose is a key feature. Aimed at gathering a better understanding of this effect, in our study this dependency was examined in more detail. To achieve this, the critical dose of a triazine-based 2D polymer[1] was measured for a wide thickness range. The polymer samples, obtained by mechanical exfoliation, ranged from 15 nm to 85 nm thickness. To obtain the critical dose of the polymer, sequences of electron diffraction patterns with a dose of only 0.5 e^-/A^2 where obtained. The measurements revealed, that the critical dose for amorphization of this polymer is only 1-2 e^-/A^2, independent of sample thickness.

References

1. F. Hu, et al. J. Am. Chem. Soc. 143, 5636-5642 (2021).

CPP 9.2 Mon 11:45 SCH A 315

Determining Anisotropic Effects in Strongly Coupled Metal Organic Hybrid Structures — •Maximilian Rödel[1], Jinhong Kim[2], Matthias Stolte[2], Luca Nils Philipp[3], Matthias Lehmann[2], Frank Würthner[2], Roland Mitric[3], and Jens Pflaum[1,4] — [1]Experimental Physics VI, University of Würzburg — [2]Institut für Organische Chemie and Center for Nanosystems Chemistry, University of Würzburg — [3]Institut für Physikalische und Theoretische Chemie, University of Würzburg — [4]Bavarian Center for Applied Energy Research, 97074 Würzburg

Coupling phenomena in metal organic hybrid structures enable unique possibilities to tune the properties of opto-electronic devices. Furthermore, the strong coupling between surface plasmons and excitons in organic semiconductors leads to novel hybrid states, which are termed plexcitons[1]. By means of a Kretschmann Set Up we investigate these plexcitonic states in oriented liquid crystalline perylene bisimide (PBI) thin films deposited via off-centered spin coating on gold surfaces which exhibiting J-type coupling [2]. The Alignment of the hydrogen-bonded PBI molecules and, thus, their transition dipoles results in long-range ordered films with a pronounced spatially anisotropy of structural and optical characteristics. These new states show a characteristic coupling strength of ≈27 meV. Understanding this directional correlation between molecular order and optical properties will enable new device concepts utilizing the presented opto-electronic directionality.

[1] Maximilian Rödel et al. J. Phys. Chem. C 2022, 126(8), 4163-4171
[2] Stefanie Herbst et al. Nat. Commun. 2018, 9(1), 2646-2654.

CPP 9.3 Mon 12:00 SCH A 315

Long-term degradation in Blatter radical derivative thin films — •Ewa Nowik-Boltyk, Tobias Junghöfer, and Maria Benedetta Casu — Universität Tübingen, Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, D-72076 Tübingen,GERMANY

Materials with a radical site are strong candidates for ground-breaking applications from energy storage to quantum computing. In this framework, Blatter radical derivatives are very attractive due to their chemical stability. We focus on the latest insights regarding the fundamental mechanisms of radical thin film long-term degradation, by comparing two Blatter radical derivatives, using X-ray-based techniques, such as photoelectron spectroscopy and absorption spectroscopy. Our findings indicate that air exposure affects the chemical and magnetic properties of the thin films.

CPP 9.4 Mon 12:15 SCH A 315

Controlled Thermal Deposition of Organic Diradicals — •Tobias Junghöfer and Maria Benedetta Casu — Institut für Physikalische und Theoretische Chemie, Eberhard Karls Universität Tübingen, Germany

Using X-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM) we demonstrate that it is possible to evaporate diradicals in a controlled environment obtaining thin films in which the diradical character is preserved. However, evaporation represents a challenge. The presence of two radical sites makes the molecules more reactive also in the case of very stable single radicals. We have explored the parameters that play a role in this phenomenon. We found that the higher the formation energies of the crystal, the more difficult is the evaporation of intact radicals. Large delocalization of the unpaired electrons helps the diradical to stand evaporation. The evaporation of different diradicals can be successfully addressed considering our findings.

CPP 9.5 Mon 12:30 SCH A 315

Interaction of cyanoacrylate thin films with copper (oxide) in different processing atmospheres — •Philipp Moritz[1], Oliver Höfft[2], Lienhard Wegewitz[1], and Wolfgang Maus-Friedrichs[1] — [1]Clausthal Centre of Material Technology, Clausthal University of Technology, Agricolastrasse 2, 38678 Clausthal-Zellerfeld — [2]Institute of Electrochemistry, Clausthal University of Technology, Arnold-Sommerfeld-Strasse 6, 38678 Clausthal-Zellerfeld

The adhesive class of fast-curing cyanoacrylates plays an increasingly important role, especially in hybrid composites. However, the adhesion mechanism at the interface to the metal (oxide) substrates is not sufficiently understood.
To study the interactions, cyanoacrylate films of a few nm thickness are spin-coated onto metallic copper and copper oxide in (i) a normal air atmosphere and in (ii) an oxygen-free environment (O_2 partial pressure $< 10^{-20}$ mbar). The natively oxidized copper is deoxidized with a dielectric barrier discharge (DBD plasma) directly before the coating process.
Spectroscopic and microscopic methods are used to understand the underlying molecular interactions at the interface between cyanoacrylate and copper (oxide). The formation of hydrogen bonds as well as an ionic interaction can be observed. In addition, an influence of the oxide layer and the effects of the surrounding atmosphere can be seen.
Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 394563137 – SFB 1368

CPP 10: Instrumentation and Methods for Micro- and Nanoanalysis (joint session KFM/CPP)

Chair: Prof. Dr. Theo A. Scherer (KIT Karlsruhe)

Time: Monday 14:30–15:30 Location: POT 106

CPP 10.1 Mon 14:30 POT 106

The Hitchhiker's Guide to BCARS on Solid-State Single Crystals — •Franz Hempel[1], Lukas König[1], Federico Vernuccio[2], Dario Polli[2], Giulio Cerullo[2], Michael Rüsing[1], and Lukas Matthias Eng[1,3] — [1]Institut für Angewandte Physik, TU Dresden, 01187 Dresden, Germany — [2]Physics Department, Politecnico di Milano, 20133 Milano, Italy — [3]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden, 01062 Dresden, Germany

Broadband coherent anti-Stokes Raman scattering (BCARS) is an advanced Raman- spectroscopy technique that offers high-speed hyperspectral imaging and is so far widely applied in the biomedical field. For crystalline materials and their high-precision analysis, however, additional aspects of phase-matching, scattering direction, and background removal delicately need to be taken into account. To prove the reproducibility of BCARS results and pinpoint setup-related influences, we have performed a comparison study using (a) two different setups, and (b) comparing transmission with epi-detection BCARS experiments. A broad set of solid-state crystalline materials with increasing complexity was analyzed, achieving comparable, background-free spectra. Also, each machine allows the specification of optimum laser and setup parameters for inspecting the different samples.

CPP 10.2 Mon 14:50 POT 106

Novel techniques for low-energy positron beam diagnostics. — •Francesco Guatieri, Michael Berghold, and Michael Zimmermann — Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Lichtenbergstr. 1, 85748 Garching, Germany

Modern surface analysis techniques based on low-energy positron annihilation require the use of a stable, focused and intense particle beam. Although several techniques are available to beam scientists to measure position, shape and intensity of a positron beam, each comes with its own limitations either in terms of precision, cost or measurement time. We will present two innovative techniques to detect low-energy positrons with the goal of performing beam optimization, each of which improves onto the previous state of the art.

CPP 10.3 Mon 15:10 POT 106

Accessible electron microscopy: Adding an EELS workflow to the ChemiTEM project — •Daniela Ramermann, Julia Menten, Elisabeth H. Wolf, and Walid Hetaba — Max-Planck-Institut für Chemische Energiekonversion, Mülheim an der Ruhr

Transmission electron microscopy is a versatile tool for the investigation of micro- and nanostructures as well as chemical and electronic properties. However, TEM experts are needed to perform the majority of analytic measurements, which represents a bottleneck in the throughput of research. To broaden access to TEM investigations for every scientist, the ChemiTEM project[1] has developed workflows for the most used techniques (HRTEM, STEM, EDX). These are implemented in an app and guide the user through every step after only a basic training.

Now a workflow for EELS measurements has been added: For the three most used measurement scenarios, assessing sample thickness, elemental mapping and oxidation state determination, a decision-tree based workflow has been created. A prerequisite is the STEM alignment from the ChemiTEM app. A set of questions about the sample evaluates if EELS measurements using the workflow are possible or a TEM expert is needed. Step-by-step instructions guarantee a standardised measurement and data quality. The workflow can be easily adapted to other microscopes and makes EELS based techniques available to a broader community.

[1] Hetaba et al., Chemistry-Methods, 1, 401-407, https://doi.org/10.1002/cmtd.202100001

CPP 11: Focus: Organic Solar Cells Based on Non-fullerene Acceptors: Loss Mechanism and Options for Above 20 % Efficiencies II

Organized by Dieter Neher and Christoph J. Brabec

Time: Monday 15:00–17:15 Location: GÖR 226

Invited Talk CPP 11.1 Mon 15:00 GÖR 226

Quantifying the potential of organic solar cells using luminescence measurements and modelling — •Jenny Nelson — Department of Physics, Imperial College London, SW7 2AZ, UK

In a molecular photovoltaic device, charge separation and energy conversion result from the evolution of a photogenerated exciton into a charge separated state, in competition with recombination to ground. Recently, new molecular materials have increased power conversion efficiency to approach 20%. To make further advances, we need to understand and isolate the effects of chemical structure, molecular packing, energetics and disorder on the competition between charge separation and recombination and hence on device efficiency. Electro- and photoluminescence have proved to be valuable tools to probe the energy and dynamics of excited states involved in photoinduced charge separation, and indirectly of the structure of molecular interfaces. Combined with other spectroscopic techniques, electrical measurements and modelling, luminescence can help us to understand how chemical and physical structure control the basic mechanisms in photovoltaic conversion. We show how such an approach can be used to study the properties and role of charge transfer states, the impact of structural and energetic disorder and to infer structure-property relationships. We apply a computational model that integrates the molecular charge transfer process with a one-dimensional drift-diffusion simulation to interpret experimental measurements and explore the effects of parameters on device performance. We consider the ultimate limits placed on solar to electric conversion by the molecular nature of the materials.

CPP 11.2 Mon 15:30 GÖR 226

Increasing the ionization offset to increase the quantum efficiency in non-fullerene acceptor based organic solar cells: How far can we go? — •Julien Gorenflot, Wejdan Alsufyani, Maryam Alqurashi, Sri Harish Kumar Paleti, Anirudh Sharma, Derya Baran, and Frédéric Laquai — KAUST Solar Center, King Abdullah University of Science and Technology, Thuwal, Kingdom of Saudi Arabia

Molecular engineering offers a virtually unlimited number of unique semiconductors for organic photovoltaics applications, that can be tailored to adapt specific needs, but only a handful of combinations enables to reach state-of-the art efficiencies. Rules are thus strongly needed to guide the design of promising systems. A recently unraveled rule is that the electron acceptor molecule requires an ionization energy 0.5 eV deeper than that of the electron donor to overcome the bending of the energy levels at the donor acceptor heterojunction interface, maximizing the charge transfer, hence the cell's quantum efficiency. Here we study the energy losses associated to this Δ IE increase. Based on 30+ blends, we show that those losses remain minimal up to an offset of 0.7 eV. We then use electroluminescence spectroscopy to evaluate the charge transfer state energy (E_{CT}) and find that this low energy losses range is associated to E_{CT} remaining at most similar to the NFA's optical bandgap ($E_{g,NFA}$), while further ΔIE increase pulls E_{CT} below $E_{g,NFA}$, accordingly decreasing V_{OC}. We finally study the evolution of the fill factor (FF) within this maximum quantum efficiency – minimal energy losses Δ IE range.

CPP 11.3 Mon 15:45 GÖR 226

The excess energy optimum to minimize recombination losses in organic solar cells — •Clemens Göhler, Alexander Flamm, and Martijn Kemerink — Institute for Molecular Systems Engineering and Advanced Materials, Universität Heidelberg, Im Neunheimer Feld 225, 69120 Heidelberg

Semiconductor blends that incorporate non-fullerene acceptors (NFA) have pushed organic solar cells to efficiency records based on an established principle: enhancing the generation yield of free charge carriers from tightly bound molecular excitations via interfacial charge transfer between donor and acceptor phases. Their success can in huge parts be attributed to an increase of the photocurrent; however, in comparison to less-effective systems, NFA blends possess a similar overall absorbance and lack the distinct low-energy absorption typically associated with charge transfer (CT) excitons.

The increased charge carrier densities are thus based on reduced recombination yields. As further improvements of the photocurrent are necessary to reach higher efficiencies, a thorough understanding of the mechanisms behind the cut in recombination losses compared to fullerene solar cells is invaluable. To contribute, we have investigated recombination signatures of both systems with respect to the available excess energy by combining field and excitation dependent electro-optical absorption spectroscopy in the steady state and close to solar cell working conditions with kinetic Monte-Carlo simulations. Our findings indicate towards an optimal excess energy which minimizes non-geminate recombination in CT processes.

CPP 11.4 Mon 16:00 GÖR 226

On the impact of the energy level offset on carrier recombination in organic non-fullerene acceptor-based solar cells — •Nurlan Tokmoldin[1], Bowen Sun[1], Floriana Moruzzi[2], Obaid Alqahtani[3], Brian Collins[3], Iain McCulloch[2], Dieter Neher[1], and Safa Shoaee[1] — [1]University of Potsdam, Potsdam-Golm, Germany — [2]University of Oxford, Oxford, UK — [3]Washington State University, Pullman, USA

The energetic offset between the highest occupied molecular orbital (HOMO) levels of the donor and acceptor components of the organic photovoltaic (OPV) blends is well-known to affect the efficiency of the singlet exciton (S1) dissociation into separated charges (CS) via the charge-transfer (CT) state, however the impact of this offset on bimolecular recombination of free charge carriers has not been explored. In this study, using three different non-fullerene acceptors Y6, ITIC and o-IDBTR, blended with the same donor polymer PM6, we demonstrate that, apart from reducing the driving force for charge generation, diminishing HOMO-HOMO energy offset also activates exciton reformation as a channel for bimolecular recombination of free charges. This is accompanied by the rise in the respective bimolecular recombination coefficient, which in turn influences the device fill-factor. Using the comparison between PM6:ITIC and PM6:o-IDBTR, we show that neither morphology, nor carrier mobilities can on their own explain the observed difference in performance, signaling the importance of the energy landscape in controlling the OPV device efficiency, both through generation and recombination of charge carriers.

15 min. break

CPP 11.5 Mon 16:30 GÖR 226

Relating free charge carrier generation and field induced photoluminescence quenching in a non-fullerene-based organic blend with a low energy offset — •Manasi Pranav[1], Thomas Hultzsch[1], Bowen Sun[1], Rong Wang[2], Safa Shoaee[1], Larry Lüer[2], Christoph Brabec[2], and Dieter Neher[1] — [1]Institute of Physics and Astronomy, University of Potsdam, 14476 Germany — [2]Institute of Materials for Electronics and Energy Technology (i-MEET), Friedrich-Alexander-Universität Erlangen-Nürnberg Martensstrasse 7, 91058 Erlangen, Germany

Many studies currently target the process of free charge carrier generation and recombination in relation to the energy level offset in organic blends based on non-fullerene acceptors (NFA). Here, we add to this discussion with a focus on the NFA Y5, characterized by a smaller highest occupied molecular orbital offset in PM6:Y5 compared to PM6:Y6, despite molecular similarity between Y5 and Y6. We find that the PM6:Y5 blend exhibits a pronounced field-dependence of free charge generation, as measured with the time-delayed collection field (TDCF) technique. We verify this with a new arbitrary-waveform TDCF technique that provides finer control over the time-delay parameters. In addition to this, we also observe a surprisingly pronounced effect of the electric field on both the steady state photoluminescence (PL) intensity and the transient PL lifetime. These results indicate that the field dependence of photo-current, free charge carrier generation and PL quenching in this low-offset system are governed by the same mechanism: likely field-induced exciton dissociation.

CPP 11.6 Mon 16:45 GÖR 226

Field Dependent Exciton Dissociation in Single-Component Organic Non-fullerene Acceptor Solar Cells — •Flurin Eisner, Mohammed Azzouzi, and Jenny Nelson — Blackett Laboratory, Imperial College London, South Kensington, SW7 2AZ, UK

Improvements in the molecular design of non-fullerene acceptors (NFAs) has almost doubled the power-conversion efficiency (PCE) of organic photovoltaics in the last 5 years, from 11 to 19%. However, the exact molecular reasons behind why some acceptors (e.g. Y-series) perform better than others (e.g. ITIC-series) remain unclear. Interestingly, recent studies have shown that some the most efficient non-fullerene acceptors can achieve relatively high charge-generation efficiency in the absence of a donor-acceptor interface, challenging the current understanding of how photogenerated excitons dissociate into free charges in organic solar cells.

Here, we study the charge-generation processes in a series of NFA molecules in single-component devices, including A-DA*D-A-type acceptors (e.g. Y6) and A-D-A type acceptors (e.g. ITIC) using optoelectronic and spectroscopy characterisation methods under strong applied fields and at different temperatures. By combining experimental results with molecular and device-level calculations, we link exciton and charge dissociation efficiency in NFA films to molecular parameters such as reorganisation energy and electronic coupling. We use this to suggest how to design materials with both higher single-component device performance and how to improve heterojunction device performance beyond 20% PCE.

CPP 11.7 Mon 17:00 GÖR 226

Triplet Excitons and associated Efficiency-Limiting Pathways in NFA-based Organic Solar Cell Blends — Jeannine Grüne[1,2], Giacomo Londi[3], Alexander J. Gillett[2], Yoann Olivier[3], Vladimir Dyakonov[1], and •Andreas Sperlich[1] — [1]Experimental Physics 6, Julius Maximilian University of Würzburg, Germany — [2]Cavendish Laboratory, University of Cambridge, UK — [3]Laboratory for Computational Modeling of Functional Materials, Université de Namur, Belgium

Organic solar cells (OSC) have made great progress in recent years, but are now reaching a performance plateau. Triplet states are known to adversely affect efficiency by opening a channel for non-radiative recombination pathways. Here, we use the complementary spin-sensitive methods of photoluminescence detected magnetic resonance (PLDMR) and transient electron paramagnetic resonance (trEPR) corroborated by transient absorption and quantum-chemical calculations to unravel exciton pathways in OSC blends employing the (non-) halogenated polymer donors PBDB-T, PM6 and PM7 together with NFAs Y6 and Y7. We reveal that all blends form triplet excitons on the NFA populated via non-geminate hole back transfer and, in blends with halogenated donors, also by spin-orbit coupling driven intersystem crossing. Identifying these triplet formation pathways in all tested solar cell absorber films highlights the untapped potential for improved charge generation to further increase efficiencies.

CPP 12: Modeling and Simulation of Soft Matter II

Time: Monday 15:00–17:15 Location: MER 02

Invited Talk CPP 12.1 Mon 15:00 MER 02

Adaptive Resolution Simulations: Past, Present and Open (Boundaries) Future — Luis A. Baptista, Mauricio Sevilla, Kurt Kremer, and •Robinson Cortes-Huerto — Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

Soft-matter systems challenge computational methods because interactions spanning a wide range of lengths and time scales require a multiscale approach capable of describing open systems and non-equilibrium conditions. Nonetheless, a high-resolution method is often only necessary to describe a relatively small portion of the system, embedded in a less detailed environment or even a particle reservoir. In this context, the adaptive resolution simulation (AdResS) method provides a seamless interpolation between high- and low-resolution descriptions: both concurrently present within the simulation box in a thermodynamically consistent framework.

In this talk, we introduce the AdResS method and present a few applications as a multiscale simulation protocol. By reducing the complexity of the low-resolution model and describing it as an ideal gas, it is practically possible to control the chemical potential of the system. In this context, we show extensions of AdResS as an efficient method to compute chemical potentials and solvation free energies in complex molecular systems. We also discuss its recent development into an open-boundary method to perform grand canonical and non-equilibrium molecular dynamics simulations. Finally, we examine possible extensions and challenges of developing the method into an open adaptive QM/MM approach.

CPP 12.2 Mon 15:30 MER 02

Chirality propagation across length scales: the case of knots in helical polymers — Yani Zhao[1], Jan Rothörl[2], Pol Besenius[3], Peter Virnau[2], and •Kostas Daoulas[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Department of Physics, Johannes Gutenberg University, Mainz, Germany — [3]Department of Chemistry, Johannes Gutenberg University, Mainz, Germany

We use computer simulations to investigate the effect of helicity in isolated polymers on the topological chirality of their knots. Polymers are described by worm-like chains (WLC), where chiral coupling between segments promotes helical conformations. The sign and magnitude of the coupling coefficient u determine the sense and strength of helicity. The excluded volume is adjusted via the radius R of a hard sphere placed at each WLC segment. Open and compact helices are, respectively, obtained for R that is zero or smaller than the length of the WLC bond, and R that is a few times larger than the bond length. We perform Monte Carlo sampling of polymer conformations for u spanning a broad range of values, from achiral polymers to polymers with well-developed helices. First, we demonstrate that the coil-helix transition in our model is not a phase transition but a crossover. Next, we perform statistical analysis of knotted polymer conformations and demonstrate that the sense of polymer helicity, left- or right-handed, influences the handedness of molecular knots and identify a generic mechanism that underlies this effect.

CPP 12.3 Mon 15:45 MER 02

Dynamics of the Rouse-mode distribution of a Gaussian chain in an external field and connection to spinodal decomposition — •David Steffen[1], Jörg Rottler[2], and Marcus Müller[1] — [1]Institut für Theoretische Physik, Georg-August-Universität, 37077 Göttingen, Germany — [2]Department of Physics and Astronomy and Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia V6T 1Z1, Canada

The current description of spinodal decomposition of a homopolymer blend via dynamic self-consistent field theory (D-SCFT) is based on the density of the monomers and uses a time-independent Onsager coefficient. This is sufficient for long wavevectors where the dynamics can be solely described by the diffusion of the center of mass. On small timescales and for larger wavevectors the dynamic is influenced by subdiffusive processes inside the chain. Therefore, a more microscopic description is needed. In this work, we provide an analytical solution for the time-dependent Rouse-mode distribution of a single chain in a weak external field. The time-dependent monomer density can then be obtained via a projection from the Rouse-mode distribution. Although different Rouse-mode distributions yield the same monomer density, an accurate description of the dynamics of the density requires the more microscopic description via the Rouse-modes distribution. This technique can be extended to the spinodal decomposition of a binary homopolymer melt. We compare the analytical results for the density and the Rouse-mode distribution to Monte-Carlo simulations of Gaussian chains.

CPP 12.4 Mon 16:00 MER 02

Simulation of diblock-copolymer membrane fabrication — •Niklas Blagojevic und Marcus Müller — Universität Göttingen, Institut für Theoretische Physik

Diblock copolymers can be used to create integral asymmetric membranes used for ultrafiltration purposes – for example water purification. The combination of evaporation-induced self assembly (EISA) and non-solvent induced phase separation (NIPS) is a promising way for efficient membrane fabrication. The importance of different time- and length-scales makes it difficult to investigate the influence of processing parameters and molecular architecture in experiments. We use a coarse-grained particle based model in conjunction with the Single-Chain in Mean Field (SCMF) algorithm to simulate membrane fabrication with EISA and SNIPS to understand how the membrane structure is formed and how it can be tailored by different processing parameters and varying molecular architecture. For example, we find that nonsolvent macrovoids in the membrane substructure coarsen with an increasing distance into the membrane, while an increasing incompatiblity between nonsolvent and polymer leads to more narrow and straight macrovoids.

15 min. break

CPP 12.5 Mon 16:30 MER 02

Salt effects on N-isopropylacrylamide in aqueous solutions. Experimental measurements, Kirkwood-Buff theory and computer simulation — Jakub Polák, •Daniel Ondo, and Jan Heyda — Department of Physical Chemistry, University of Chemistry and Technology, Prague, Technická 5, 166 28 Prague 6, Czech Republic

In this work, we investigate salt-specific effects on N-isopropylacrylamide (NiPAM) by means of densimetry and vapor pressure osmometry, employing family of sodium and guanidinium salts from low NiPAM concentration up to the solubility limit. Employing Kirkwood-Buff (KB) theory, complete set of effective pair interactions, KB-integrals, at any composition are determined, serving as a bridge to well calibrated molecular dynamics (MD) simulation. All atom MD simulations were used in direct analogy to the experiments and volumetric properties determined. For the first time, in-silico vapor pressure osmometry experiment was performed and excess osmolality evaluated from ternary solution structure. Finally, we establish a strong correlation between salt effect on NiPAM hydration and the salting-out ability of studied salts.

CPP 12.6 Mon 16:45 MER 02

Evaporation-induced confinement assembly of functional terpolymer microparticles — •Elias M. Zirdehi[1], Manuel Trömer[2], André H. Gröschel[2], and Arash Nikoubashman[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz — [2]Institute of Physical Chemistry, University of Münster

Evaporation-induced confinement assembly of terpolymers is an effective technique for fabricating internally structured microparticles (MPs). The wide range of usable building blocks allows for a large variety of MPs, but poses also an immense challenge due to the staggering amount of process parameters, which cannot be explored through experiments alone. Therefore, we performed dissipative particle dynamics simulations of a bead-spring model to study the directed assembly of triblock copolymers in evaporating droplets. We developed a semi-grand canonical simulation approach, where droplet particles in the vapor phase are periodically removed to drive evaporation at constant flux. In this model, the evaporation rate is controlled by the frequency and the number of particle removal. The resulting shrinking of the droplet was in excellent agreement with theory and experiments. We then implemented this procedure to investigate how the final morphology of terpolymer MPs is influenced by the evaporation rate as well as surfactant type. Finally, the possibility of altering the morphology tailored for specific applications by adding homopolymers will be discussed.

CPP 12.7 Mon 17:00 MER 02

Wavenumber dependent viscosity of a system of particles coupled dissipatively to a Lattice Boltzmann fluid — •Joydip Chaudhuri[1] and Burkhard Dünweg[1,2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Department of Chemical and Biological Engineering, Monash University, Clayton, Victoria 3800, Australia

We consider a particle based Molecular Dynamics (MD) system coupled dissipatively to a stochastic Lattice Boltzmann (LB) fluid. The employed force coupling method is dissipative which means that the velocity of an MD particle is damped with respect to the velocity of the LB fluid interpolated to the position of the particle. The present study explores the viscosity response of such a coupled LBMD system due to a sinusoidally varying external force. The analytic theory for that system is based upon a two-fluid model, whose predictions are well corroborated by numerical tests. Except for the respective viscosities of the two uncoupled fluids, the total viscosity of the coupled system depends on a hydrodynamic screening length associated with the Stokes coupling parameter, the mass density ratio, and the wavenumber of the applied external force. In the asymptotic long-wavelength limit, the total viscosity is just the sum of the two input viscosities. This behavior deviates significantly from the well known Einstein prediction for dilute colloidal dispersions, and this is due to the different type of particle-fluid coupling.

CPP 13: Composites and Functional Polymer Hybrids

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

Invited Talk CPP 13.1 Mon 15:00 ZEU 255

Nanocomposites and polymer thin films: from gas phase synthesis to functional applications — •Franz Faupel, Stefan Schröder, Alexander Vahl, Salih Veziroglu, Cenk Aktas, and Thomas Strunskus — Chair for Multicomponent Materials, Faculty of Engineering, Kiel University, Kiel, Germany

Highly filled particulate metal-dielectric nanocomposites films have unique functional properties with hosts of applications. To explore collective interactions between the particles, we control the particle separation on the nm scale by employing vapor phase deposition, which is a scalable approach permitting, inter alia, excellent control of the filling factor. For deposition of functional polymer thin films, we have recently used initiated chemical vapor deposition (iCVD) to avoid decomposition of the functional groups. Examples include highly stable electrets for electret microphones and magnetoelectric sensors, 3D superhydrophobic coatings, nanoscale gradient copolymers, and strain-invariant conductors for soft robotics. For the fabrication of the nanocomposites, the nanoparticles can form during gas phase co-deposition via self-organization or by means of high-rate gas aggregation cluster sources, which provide independent control of filling factor and size as well as in situ monitoring and control of composition. Recent examples of nanocomposites range from plasmonic meta-materials through photoswitchable molecular plasmonic systems to memristors and memsensors for neuromorphic electronics. We also explored nanoscale synergetic effects of plasmonics and photocatalysis, e.g. for photoinduced enhanced Raman spectroscopy (PIERS).

CPP 13.2 Mon 15:30 ZEU 255

Rheological optimization of filler packings using micro scale simulations — •Oliver Roser[1,2], Andreas Griesinger[3], and Othmar Marti[2] — [1]Center for Heat Management (ZFW), Stuttgart — [2]Institute of Experimental Physics, Ulm University — [3]Baden-Wuerttemberg Cooperative State University (DHBW) Stuttgart

In a wide range of applications, polymers are modified with granular fillers to improve thermal or electric conductivity. The higher the amount of filler, the higher the conductivity. However, the attainable conductivity is restricted by processing limitations as the amount of filler also affects the composites viscosity. Only a clever combination of filler with multimodal size distributions can shift this limit and allow for higher amounts of filler without significant viscosity increase. The effect of multimodal packing structures on viscosity has already been investigated in several experimental and numerical studies, however common calculation techniques are mainly restricted to spherical and equal-sized filler particles. We extended common approaches with new packing simulations, considering the actual size distribution and shape of different filler materials. We implemented numerical packing optimization to find the best filler compositions for highly filled polymers with up to 80 v%. In this talk we will introduce the new packing simulations and their use for packing optimizations and present the acquired results and experimental validations.

CPP 13.3 Mon 15:45 ZEU 255

Increasing the Electrical Conductivty of Polymer Thin Films for Thermoelectric Applications — •Marie Siegert[1], Markus

Hönig[2], Michael Sommer[2], and Jens Pflaum[1,3] — [1]University of Würzburg — [2]Chemnitz University of Technology — [3]ZAE Bayern

Thermoelectric generators based on sustainable, low-cost organic materials harbor great potential for waste heat recovery. Polymer thin films in particular can be easily upscaled to meet industrial standards and display aptly low thermal conductivity κ, but lack high electrical conductivity σ. However, the augmentation of σ imposes a major challange as an increase in charge carrier concentration is usually accompanied by an unintentional decrease of the Seebeck coefficient S, which is detrimental for efficient thermoelectrics. Hence, we compare two possible strategies to enhance the charge carrier transport in such disordered systems. Firstly, doped polymer thin films utilizing the temperature activated n-type dopant TAM have been characterized regarding their thermoelectric properties. Secondly, composite films have been investigated, combining well studied polymers with metallic additives. Both approaches will be evaluated with respect to the enhancement in σ and the underlying transport mechanisms. First estimations of the resulting power factors indicate future strategies to further refine the electronic properties and thus, the thermoelectric figure of merit.
The Deutsche Bundesstiftung Umwelt (DBU) is acknowledged for financial support.

CPP 13.4 Mon 16:00 ZEU 255

Conductivity of filled diblock copolymer systems. — •Alexander Chervanyov — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Münster, Germany

The reported work looks into the effect of stimuli-induced morphological changes in the composite consisting of insulating diblock copolymers (DBC) and conductive nanoparticles (NP) on the conductivity of this composite. The relation between the nano-structure of the described composite and its conductivity is studied by developing and making use of the multiscale computational approach. This approach relies on the consistent phase-field model of DBC, Monte-Carlo simulations of the filler distribution in DBC, and the resistor network model of the composite conductivity. The dependencies of the conductivity on the temperature of the composite, DBC morphology, and the affinities of fillers for copolymer blocks are studied in detail. In particular, the order-disorder transition in the host DBC system is found to be accompanied by the conductor-insulator transition in the filler network. The order-order transition between the lamella and cylindrical microphases of DBC proves to co-occur with a spike of the composite conductivity caused by restructuring of the conductive filler network.

15 min. break

CPP 13.5 Mon 16:30 ZEU 255

Modeling micro-structure evolution and its impact on moduli in magneto-active elastomers — •Mehran Roghani, Dirk Romeis, and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden, Germany

Magneto Active Elastomers (MAEs) are field-controllable composites made of micron-sized, magnetizable particles embedded into a soft elastomeric matrix. These materials show a strong coupling between their mechanical properties and an applied magnetic field. The coupling can be directly related to magnetic interactions between the particles, which lead to the evolution of microstructure under the field. In the case of initially isotropic MAEs, this micro-structure evolution results in chains forming from the magnetized particles. This in turn causes a huge increase in the mechanical moduli along the field direction, leading to anisotropic behavior. We consider a transversely isotropic material model for the mechanics, and magnetic interactions are taken into account by the dipolar mean field approach. To couple the mechanical and magnetic effects, a restructuring parameter is introduced which is a function of material magnetization and moduli. This modeling approach improves our understanding of how microstructure evolution affects magnetically induced material deformation and stiffness. The first predictions are in good agreement with experimental results available in the literature. We thank the DFG for financial support through RTG-2430.

CPP 13.6 Mon 16:45 ZEU 255

Magneto-active elastomers: From composite structure to effective susceptibility — •Dirk Romeis and Marina Saphiannikova — Leibniz-Institute of Polymer Research Dresden e.V.

Embedding magnetizable particles into elastic polymer network yields a field-controllable material known as magneto-active elastomer (MAE). In order to describe macroscopic samples of such composite material it is useful to develop an effective macro-continuum model. Based on the dipole approximation, we derive analytic relations for the effective magnetization behavior in MAEs, spanning from linear to saturation regime, for isotropic and anisotropic particle arrangements. In the limiting case of linear magnetics and isotropic distributions we reproduce an expression known from previous works. Accordingly, we believe that the present homogenization scheme provides a general description of the effective magnetic behavior with high practical relevance also in case of anisotropic distributions and beyond the linear magnetization. For a given particle arrangement and magnetization model on microscale, the solutions are obtained with low computational effort. Furthermore, the present formulation can be directly implemented into a macroscopic material model for a composite sample of specified shape. It turns out, that an anisotropic particle distribution has an equivalent effect as an anisometric sample shape.

CPP 13.7 Mon 17:00 ZEU 255

Tuning the thermal conductivity of magnetic gels and elastomers — Gustav J. L. Jäger, •Lukas Fischer, Tyler Lutz, and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

When an external magnetic field is applied to magnetic gels or elastomers—composite materials consisting of magnetic or magnetizable particles inside an elastic matrix—these materials typically exhibit interesting deformational (magnetostrictive) responses or changes in rheological properties (magnetorheological effect).

We study how the induced magnetic interactions lead to an internal restructuring of the magnetic particles, mainly the formation of particle chains along the direction of the external magnetic field. This behavior is not only connected to the aforementioned effects, it can also change the thermal conductivity of the magnetic gels and elastomers, which we focus on here. We analyze this phenomenon numerically for 2D mesoscopic (particle-resolved) models of magnetic gels and elastomers [1], thus characterizing thin elastic films and membranes.

Our results indicate significant magnetically induced changes in the thermal conductivity. The influence of several parameters on this effect is investigated, such as the density and number of magnetizable particles, the amplitude of their magnetization, and the aspect ratio of the systems. Similar changes in the electric conductivity of magnetic gels and elastomers are expected.
[1] G. J. L. Jäger, L. Fischer, T. Lutz, A. M. Menzel, J. Phys.: Condens. Matter **34**, 485101 (2022).

CPP 13.8 Mon 17:15 ZEU 255

Morphology evolution and nanoparticle localization in printed hybrid nanoparticle-diblock copolymer thin films investigated by in situ GISAXS — •Christopher R. Everett[1], Guangjiu Pan[1], Manuel A. Reus[1], David Kosbahn[1], Frank Hartmann[2], Martin Bitsch[2], Matthias Opel[3], Markus Gallei[2], Matthias Schwartzkopf[4], and Peter Müller-Buschbaum[1,5] — [1]TUM, TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching — [2]Saarland University, LS Polymer Chemistry, 66123 Saarbrücken — [3]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — [4]DESY, 22607 Hamburg — [5]MLZ, TUM, 85748 Garching

The diblock copolymer (DBC) PS-b-PMMA forms films with periodic ordered nanostructures that can act as scaffolds for inorganic magnetic nanoparticles. These films have application as magnetic sensors and in magnetic data storage devices. Film formation and the resulting magnetic properties both depend on the localization of the nanoparticles in the DBC domains. In this investigation, ultra-high molecular weight PS-b-PMMA films containing two types of nanoparticles, cobalt ferrite and nickel, are fabricated by a slot-die coating technique. Grazing incidence small-angle X-ray scattering (GISAXS) is used to monitor in situ the morphological evolution of the DBC films and nanoparticle segregation in the films during the deposition and drying process. The magnetic properties of the hybrid films are investigated with a SQUID magnetometer.

CPP 13.9 Mon 17:30 ZEU 255

Tunable mesoporous zinc titanate films via diblock copolymer-directed cooperative self-assembly and a sol-gel technique — •Yanan Li[1], Nian Li[1], Shanshan Yin[1], Constantin Harder[2], Yusuf Bulut[2], Apostolos Vagias[3], Stephan V. Roth[2,4], and Peter Müller-Buschbaum[1,3] — [1]TUM School of

Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]DESY, 22607 Hamburg, Germany — [3]MLZ, TUM, 85748 Garching, Germany — [4]Department of Fiber and Polymer Technology, KTH, SE-100 44 Stockholm, Sweden

Mesoporous ordered films have broad applications ranging from sensors to supercapacitors and biodevices due to their large specific surface area and pore accessibility of their porous nanostructures. Here, we investigate the evolution and formation mechanisms of morphologies of mesoporous zinc titanate films obtained by changing the ratio of two inorganic precursors after calcining hybrid films consisting of organic-inorganic materials. The amphiphilic diblock copolymer self-assembles into micelles in a mixture of N,N-dimethylformamid/hydrogen chloride playing the role as structure directing template. The inorganic precursors are loaded in the micellar shell due to hydrogen bonds between PEO and precursors. We combine a sol-gel route with a spin coating to prepare hybrid films, and investigate the influence of the different weight fractions of precursors and polymer concentration on the film morphologies. The inner and surface morphologies of the hybrid films are characterized using grazing incidence small-angle X-ray scattering and scanning electronic microscopy, respectively.

CPP 13.10 Mon 17:45 ZEU 255

Gold Nanoparticle/Polymer Brushes Composites: Controlling the Structure via Ion-Specific Effects — •Philipp Ritzert and Regine v. Klitzing — Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany

Nanocomposite materials based on inorganic gold nanoparticle (AuNP) inclusions inside an organic matrix (e.g. polymer brushes) are employed in various fields: medical technology, catalysis, materials engineering. Combining the properties of both material classes facilitates high versatility of mechanical, optical and chemical properties, while simultaneously covering obvious drawbacks, e.g. stability of one compound. To provide the wide range of applications, nanocomposite materials usually require a specific internal structure. Yet, the understanding of the formation of internal structure and control over formation process is still lacking. Therefore, we aim to provide an approach to manufacture nanocomposite materials with controlled structure. Our model system utilizes various sodium salts (anion: F, Cl, Br, I, SCN) as stimuli for the assembly of citrate-capped gold nanoparticles in a poly-(N-isopropylacrylamide) brush. In a first step, we characterize the effect of sodium salts on pure AuNP suspensions. In a second step, we investigate adsorption parameters of AuNPs from suspension to brush, e.g. adsorption time. The third step involves the structure control of the composite materials with the characterized stimuli. Optical measurements reveal distinct differences between the sodium ions and concentration dependent aging behaviour.

CPP 14: Active Matter II (joint session DY/BP/CPP)

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

CPP 14.1 Mon 15:00 ZEU 160

Chiral motion of actively driven objects in discrete steps towards a remote target — •Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

We address the motion of chiral actively driven objects that move in discrete steps on a flat substrate [1]. While closed polygon-shaped trajectories are found in the case of unperturbed motion, the dynamics becomes surprisingly rich and nonlinear, if the objects additionally head for a fixed remote target. In that situation, cycloidal-like, straight, zigzag-type, doubled zigzag, quadrupled zigzag, and further period-doubled types of trajectory emerge, besides chaotic behavior. Additionally, we investigate the motion of crowds of such objects under explicit mutual alignment interaction. In the absence of fluctuations, collective orientational ordering occurs also in the chaotic regime, in combination with spatial gathering of the particles. Conversely, fluctuations and polydispersity in target alignment counteract orientational ordering. Our results may apply to various types of actively driven objects, for instance, light-responsive bacteria, laser-controlled colloidal particles, or hoppers on vibrated substrates.

[1] A. M. Menzel, resubmitted.

CPP 14.2 Mon 15:15 ZEU 160

Polar flocks with discretized directions: the active clock model approaching the Vicsek model — •Matthieu Mangeat, Swarnajit Chatterjee, and Heiko Rieger — Universität des Saarlandes, Saarbrücken, Germany

We study the off-lattice two-dimensional q-state active clock model (ACM) [EPL **138**, 41001 (2022)] as a natural discretization of the Vicsek model (VM) [PRL **75**, 1226 (1995)] describing flocking. The ACM consists of particles able to move in the plane in a discrete set of q equidistant angular directions, as in the active Potts model (APM) [EPL **130**, 66001 (2020); PRE **102**, 042601 (2020)], with a local alignment interaction inspired by the ferromagnetic equilibrium clock model. A collective motion emerges at high densities and low noise. We compute phase diagrams of the ACM and explore the flocking dynamics in the region, in which the high-density (polar liquid) phase coexists with the low-density (gas) phase. We find that for a small number of directions, the flocking transition of the ACM has the same phenomenology as the APM, including macrophase separation and reorientation transition from transversal to longitudinal band motion as a function of the particle self-propulsion velocity. For a larger number of directions, the flocking transition in the ACM becomes equivalent to the one of the VM and displays microphase separation and only transverse bands, i.e. no reorientation transition. Concomitantly also the transition of the $q \to \infty$ limit of the ACM, the active XY model, is in the same universality class as the VM. We also construct a coarse-grained hydrodynamic description akin to the VM.

CPP 14.3 Mon 15:30 ZEU 160

Tracer-induced temperature difference in motility-induced phase separation — •Lukas Hecht, Iris Dong, and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstr. 8, D-64289 Darmstadt, Germany

Previous studies of overdamped active Brownian particles (ABPs) mixed with passive tracers have shown that self-propulsion can induce motility-induced phase separation (MIPS) for large enough particle density and self-propulsion speed [1]. Here, we present our study on overdamped ABPs mixed with inertial passive tracers. We show that MIPS features different kinetic temperatures in the dense and the dilute phase if the passive tracers are sufficiently heavy (inertial). Remarkably, unlike for underdamped ABPs [2,3], neither the overdamped ABPs nor the passive tracers alone would feature such a temperature difference in coexisting phases. The observed temperature difference is accompanied by a violation of the equipartition theorem and strongly depends on the self-propulsion speed and the particle density. This allows us to tune the temperature difference from a cold dense and hot dilute phase to the counterintuitive opposite case in which the dense phase is hotter than the dilute phase. These findings open a route to create active materials with a persistent temperature profile by inserting active particles and tuning their self-propulsion speed accordingly.

[1] J. Stenhammar et al., Phys. Rev. Lett. 114, 018301 (2015).
[2] S. Mandal et al., Phys. Rev. Lett. 123, 228001 (2019).
[3] L. Hecht et al., Phys. Rev. Lett. 129, 178001 (2022).

CPP 14.4 Mon 15:45 ZEU 160

Collective motion in two-dimensional colloidal systems with effective (active) self-propulsion due to time-delayed feedback — •Robin A. Kopp and Sabine H. L. Klapp — ITP, TU Berlin, Berlin, Germany

In recent years, delayed feedback in colloidal systems has become an active and promising field of study [1,2], key topics being history dependence and the manipulation of transport properties. Here we study the dynamics of a two-dimensional colloidal suspension, subject to time-delayed feedback, where time-delayed feedback can be interpreted as a mechanism of effective self-propulsion, i.e., activity [3]. To this end we perform overdamped Brownian dynamics simulations, where the particles interact through a Weeks-Chandler-Andersen potential. Furthermore, each particle is subject to a Gaussian, repulsive feedback potential, that depends on the difference of the particle position at the current time, and at an earlier time. We observe and quantitatively study the emergence of dynamical clustering and collective motion characterized by a nonzero mean velocity and provide a possible explanation for the underlying mechanism combining single-particle and mean-field-like effects.

[1] S. A. M. Loos, and S. H. L. Klapp, Scientific Reports **9**, 2491 (2019)
[2] M. A. Fernandez-Rodriguez et al., Nature Communications **11**, 4223 (2020)
[3] R. A. Kopp and S. H. L. Klapp, arXiv:2210.03182 (2022)

CPP 14.5 Mon 16:00 ZEU 160

Inverted Sedimentation of Active Particles in Unbiased ac Fields — •José Carlos Ureña Marcos and Benno Liebchen — Institut für Physik Kondensierter Materie, TU Darmstadt, Darmstadt, Germany

Biological microswimmers can steer autonomously and use this ability to perform sophisticated tasks. Synthetic microswimmers do not yet reach the same degree of autonomy, and need to be controlled externally if they are to carry out tasks such as targeted cargo delivery or microsurgery. While much progress has been made recently to control their motion based on external forces or gradients, e.g. in light intensity, which have a well-defined direction or bias, little is known about how to steer APs in situations where no permanent bias can be realized.

Here, we show that ac fields with a vanishing time average provide an alternative route to steering APs. We exemplify this route for inertial APs in a gravitational field, observing that a substantial fraction of them persistently travels in the upward direction upon switching on the ac field, resulting in an inverted sedimentation profile at the top wall of a confining container. Our results offer a generic control principle which could be used in the future to steer active motion, to direct collective behaviors and to purify mixtures.

15 min. break

Invited Talk CPP 14.6 Mon 16:30 ZEU 160

Long-range communications enable the hierarchical self-organization of active matter — •Igor Aronson[1], Alexander Ziepke[2], Ivan Maryshev[2], and Erwin Frey[2] — [1]Pennsylvania State University, USA — [2]Ludwig-Maximilians-University, Munich, Germany

The most distinct markers of life are the ability to move (locomotion), consume energy (metabolism), process information, and form multi-cellular aggregates. Many biological systems exhibit long-range signaling strategies for evolutionary advantage. We explore the multiscale self-organization of interacting self-propelled agents that locally process information transmitted by chemical signals. The communication capacity dramatically expands their ability to form complex structures, allowing them to self-organize through a series of collective dynamical states at multiple hierarchical levels.

The consequent study shows that information exchange by acoustic waves between the self-propelled units creates a slew of multifunctional structures. Each unit is equipped with an acoustic emitter and a detector in this realization. The swarmers respond to the resulting acoustic field by adjusting their emission frequency and migrating toward the strongest signal. We find self-organized structures with different morphology, including snake-like self-propelled entities, localized aggregates, and spinning vortices. Our results provide insights into the design principles of communicating active particles capable of performing complex tasks.

CPP 14.7 Mon 17:00 ZEU 160

Arrested by heating — •Corinna C. Maass[1,2], Prashanth Ramesh[2,1], and Maziyar Jalaal[3] — [1]University of Twente, Enschede, Netherlands — [2]MPI for Dynamics and Self-organization, Göttingen, Germany — [3]Universiteit van Amsterdam, Amsterdam, Netherlands

Active droplets are a class of microswimmers driven by chemical reactions at the droplet interface. Typically, the activity is powered by an advection-diffusion instability in the chemohydrodynamic fields around the droplet that is characterised by the Péclet number Pe of chemical transport. With increasing Pe, higher hydrodynamic modes at the interface cause the droplet to transition from inactivity, to steady, to reorienting, to fully unsteady motion. Here, we demonstrate that it is possible to change Pe reversibly and in situ by thermally activated changes in the chemical enviroment, and thereby to control the motility of the droplet.

CPP 14.8 Mon 17:15 ZEU 160

Chiral active particles with non-reciprocal couplings: results from particle-based simulations — •Kim L. Kreienkamp and Sabine H. L. Klapp — Technische Universität Berlin, Germany

Non-reciprocal interactions manifest their drastic impact on the collective dynamics of active matter systems by changing, for example, the general type of observed instabilities [1] and leading to time-dependent states [2,3]. In particular, the combination of non-reciprocity and chirality in terms of intrinsically rotating chiral active particles ("circle swimmers") reveals intriguing non-trivial time-dependent collective dynamics [1].

After having developed an understanding of the collective dynamics on the continuum level in previous work [1], we here present first results of particle-based simulations of chiral active particle systems with non-reciprocal alignment couplings. Indeed, quantitative predictions from continuum approaches are somewhat limited by the approximations made during the coarse-graining process. Thus, the first goal of our particle-based simulations is to explore the validity of the previously obtained continuum results regarding the overall state diagram. Second, we aim at investigating microscopic aspects of the various time-dependent states. Finally, we discuss possibilities to characterize the thermodynamic behavior of the non-reciprocal chiral system based on the stochastic trajectories obtained in particle-resolved simulations.

[1] K. L. Kreienkamp and S. H. L. Klapp, New J. Phys. (2022).
[2] M. Fruchart et al., Nature 592, 363 (2021).
[3] Z. You et al., PNAS 117, 19767 (2020).

CPP 14.9 Mon 17:30 ZEU 160

Lattice-induced freezing in active systems unveils dynamic crystallites with square ordering — •Aritra K. Mukhopadhyay[1], Peter Schmelcher[2,3], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, 64289 Darmstadt, Germany. — [2]Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany. — [3]The Hamburg Centre for Ultrafast Imaging, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany.

Active matter, comprising self-propelled particles like bacteria, colloidal microswimmers, or granular microflyers is currently attracting enormous attention for its ability to self-organize into complex nonequilibrium structures. In this work, we report on a new state of dynamic active crystallites, which occurs when exposing active particles to a spatially periodic potential. These crystallites require activity to emerge, adopt the structure of the underlying lattice (e.g. square rather than hexagonal close packing), and are continuously in motion. This new phase unifies the structural properties of crystals with the dynamical properties of disordered fluids. Our work thus unveils a route to creating a new state of active materials with an intrinsic structure that can be externally controlled.

CPP 14.10 Mon 17:45 ZEU 160

Shape-dependent collective motion: cohesive groups and cargo transport of colloidal rods — Philipp Stengele, •Anton Lüders, and Peter Nielaba — Universität Konstanz, Konstanz, Deutschland

In active toy model systems where colloids interact via predefined social interaction rules as well as steric collisions, the shape of the individual particles strongly influences emerging collective behavior. We study this based on two example systems using Brownian dynamics simulations (without hydrodynamic interactions). Firstly, we investigate a simple perception model in which colloidal rods move actively if predefined visual stimuli exceed a certain threshold. Here, we find an aspect ratio range where the rods form a dilute cohesive group with a time-independent particle distribution. If the aspect ratio surpasses this range, the rods slowly drift apart. Secondly, we look into the cargo capture and transport of a passive rod using a dense swarm of active spheres which form a hexagonal cage with a cavity for the cargo. Again, the aspect ratio of the rod proves to be crucial, as we find geometric restrictions that must be met to stabilize the cavity. Our work underlines that the shape (here, the aspect ratio) of the particles in active matter systems must be carefully considered while defining interaction rules to perform specific tasks.

CPP 14.11 Mon 18:00 ZEU 160

Active Chiral Nematics — •Rüdiger Kürsten[1,2,3] and Demian Levis[1,2] — [1]Departament de Física de la Matèria Condensada, Universitat de Barcelona, Barcelona, Spain — [2]Universitat de Barcelona Institute of Complex Systems (UBICS), Barcelona, Spain — [3]Institut für Physik, Universität Greifswald, Greifswald, Germany

We study inherently chiral self-propelled particles in two dimensions that are subjected to nematic alignment interactions and rotational noise. By means of both, homogeneous and spatially resolved mean field theory we identify various different flocking states. We confirm the presence of the predicted phases using agent-based simulations. We emphasize that special care has to be taken within the simulations in order to avoid artifacts. We present a non-standard simulation technique in order to avoid those artifacts.

CPP 15: 2D Materials II (joint session HL/CPP)

Time: Monday 15:00–18:15 Location: POT 81

CPP 15.1 Mon 15:00 POT 81

Twist- and gate-tunable valley splitting in TMDC/$\mathrm{CrI_3}$ heterostructures — •Klaus Zollner, Paulo E. Faria Junior, and Jaroslav Fabian — Institute of Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany

Van der Waals heterostructures composed of twisted monolayers promise great tunability of electronic, optical, and magnetic properties. Twistronics has already demonstrated its potential in tuning proximity spin-orbit and exchange coupling in graphene-based heterostructures [1,2]. In this talk, we present the strong manipulation of the valley splitting upon twisting and gating in TMDC/$\mathrm{CrI_3}$ heterostructures [3]. In particular, upon twisting from 0° to 30°, the proximity-induced TMDC valence band edge exchange splitting can be reversed (-2 to 2 meV), while the TMDC conduction band edge exchange splitting remains nearly constant (-3 meV). Further giant tunability (few meV) of the proximity exchange coupling is provided by a transverse electric field. Consequently, twisting and gating then allow to tailor the valley splitting of the first intralayer exciton peak in the range of 0 to 12 meV in $\mathrm{WSe_2/CrI_3}$, which is equivalent to gigantic external magnetic fields of up to about 60 Tesla.

This work was supported by DFG SFB 1277, DFG SPP 2244, and the EU Horizon 2020 Research and Innovation Program (Graphene Flagship).

[1] K. Zollner and J. Fabian, Phys. Rev. Lett. 128, 106401 (2022).
[2] Lee *et al.*, Phys. Rev. B 106, 165420 (2022).
[3] K. Zollner, P. E. F. Junior, J. Fabian, arXiv:2210.13794 (2022).

CPP 15.2 Mon 15:15 POT 81

Giant Enhancement of Interlayer Exciton Luminescence in $\mathrm{WSe_2/WSe_2/MoSe_2}$ in Heterotrilayers. — •Chirag Palekar, Ching-Wen Shih, Imad Limame, Bárbara Rosa, and Stephan Reitzenstein — Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany

TMDC heterolayers have gained lot on interest as a promising platform to study intricate many-body physics phenomena. Here we observe giant enhancement of interlayer exciton PL in a $\mathrm{WSe_2/WSe_2/MoSe_2}$ heterotrilayers (HTL) system prepared by employing exfoliation and dry transfer method. The IX exciton forming at the heterojuction in the HTL region exhibits 10-fold increase in PL yield when compared to HBL region on the same sample. Such an enhancement can be attributed to the close to 0^0 twist angle between stacked $\mathrm{WSe_2}$ homobilayers providing smaller interlayer separation and hybridization in the $\mathrm{WSe_2}$ band structure, which in turn results in an efficient charge transfer. Further, PLE and reflection contrast reveal the twist angle dependence of the enhancement factor in such type II HTL systems as the large twist angel between $\mathrm{WSe_2}$ homobilayers (57^0) results in only up to 10% percent enhancement of IX PL in the HTL region when compared with the HBL. This fundamental study of excitons in the HTL system deepens the current understanding of physics of twisted TMDC heterostructures and paves the way for future experiments and theoretical work.

CPP 15.3 Mon 15:30 POT 81

Photoluminescence tuning in hybrid devices of monolayer transition metal dichalcogenides and rylene dyes — •Theresa Kuechle[1], Gergely Knorr[2], Kalina Peneva[2], and Giancarlo Soavi[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Institute of Organic Chemistry and Macromolecular Chemistry, Friedrich Schiller University Jena, Lessingstraße 8, 07743 Jena, Germany

Monolayer transition metal dichalcogenides (TMDs) are direct gap semiconductors that hold great promise for applications in nanoscale photonics and optoelectronic devices. A viable path for the development of devices with advanced functionalities and tunable properties is the integration with other nanoscale systems such as nanowires [1] and molecules [2]. Here, we realize hybrid devices based on TMDs and rylene dyes and study their optical properties via steady state photoluminescence. Preliminary results show that the PL emission in hybrid structures of $\mathrm{WS_2/CN_4PMI}$ can be quenched by a factor of 3, in the case of $\mathrm{WSe_2/CN_4PMI}$ by 300. We tentatively assign this variation to a different band alignment in the two heterostructures and to the interplay between charge transfer (in type II) and energy transfer (in type I). Future experiments including ultrafast pump-probe spectroscopy of pristine and hybrid systems as well as hybridization of different (tunable) molecules will further elucidate the role of band alignment in the ultrafast charge and energy transfer processes at the nanoscale.

[1] Kim *et al.*, *ACS Nano* **14**, 9, 4323 (2020)
[2] Park *et al.*, *Adv. Mat. Interfaces* **8**, 12, 2100215 (2021)

CPP 15.4 Mon 15:45 POT 81

Coherence of interlayer exciton ensembles in $\mathrm{MoSe_2/WSe_2}$ heterobilayers — •Christos Paspalides[1], Mirco Troue[1], Johannes Figueiredo[1], Lukas Sigl[1], Manuel Katzer[2], Malte Selig[2], Andreas Knorr[2], Ursula Wurstbauer[3], and Alexander Holleitner[1] — [1]TU Munich — [2]Technische Universität Berlin — [3]University of Münster

Transition metal dichalcogenides exhibit strong light-matter interactions, which suggests them to be ideal candidates for novel 2D optoelectronic applications. Corresponding van der Waals heterostacks allow the excitation and formation of long-lived interlayer excitons [1]. We present coherence measurements of the ground state in such interlayer exciton ensembles by performing Michelson-Morley interferometry over a wide range of exciton density and temperature [2]. Moreover, we discuss the expansion dynamics of the interlayer excitons presumably driven by dipole-dipole interactions. The presented work paves the way towards a detailed understanding of excitonic many-body quantum phenomena in two-dimensional materials [3].

[1] B. Miller et al., Nano Letters 17, 5229 (2017).
[2] M. Troue and J. Figueiredo, et al (2023).
[3] L. Sigl et al., Signatures of a degenerate many-body state of interlayer excitons in a van der Waals heterostack, Phys. Rev. Res. 2, 042044 (2020).

15 min. break

CPP 15.5 Mon 16:15 POT 81

Theoretical description of interlayer excitons in TMD homobilayers — •Ruven Hübner[1], Alexander Steinhoff[1], and Matthias Florian[2] — [1]Institut für Theoretische Physik, Universität Bremen, Bremen, Germany — [2]University of Michigan, Dept. of Electrical Engineering and Computer Science, Ann Arbor, MI, USA

In recent years, interlayer excitons in bilayers of transition metal dichalcogenides (TMDs) have received a rapid increase in attention. On the one hand, they feature the main characteristics of conventional excitons in the corresponding monolayers, namely an absorption spectrum in the optical regime combined with a high binding energy. On the other hand, they differ to such intralayer excitons by a massively increased life time, a non-zero dipole moment in the out-of-plane direction and a strong sensitivity to material combination as well as stacking arrangement of adjacent monolayers. In this talk we focus on special excitonic properties inside TMD homobilayers that are particularly demanding from a theoretical point of view. In this context we discuss moiré excitons in twisted bilayers as well as high-lying excitons and trions at around twice the band gap energy arising within a highly non-parabolic band dispersion.

CPP 15.6 Mon 16:30 POT 81

Raman signature of interlayer coupling and lattice dynamics in 2D TMDCs — •Yang Pan[1,2] and Dietrich R. T. Zahn[1,2] —

[1]Semiconductor Physics, Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Center for Materials, Architectures, and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany

Vertical stacking of two-dimensional (2D) homo- and heterostructures are intriguing research objects, as they are essential for fundamental studies and a key towards 2D device applications. It is paramount to understand the interlayer coupling in 2D materials and to find a fast yet precise characteristic signature. In this work, we report on a Raman fingerprint of interlayer coupling in 2D transition metal dichalcogenides (TMDCs). We observed that the out-of-plane B_{2g} vibrational mode is absent when two monolayers form a vertical stack yet remain uncoupled but emerges after strong coupling. Using systematic Raman, photoluminescence (PL), and atomic force microscopy (AFM) studies of WSe_2/WSe_2 homo-bilayers and $MoSe_2/WSe_2$ hetero-bilayers, we conclude that the B_{2g} vibrational mode is a distinct Raman fingerprint of interlayer coupling in 2D TMDCs. Our further investigations confirmed its applicability on twisted 2D homo- and hetero-bilayers. Our results propose an easy, fast, precise, and reliable measure to evaluate the interlayer coupling and twisting angles in 2D TMDCs.

CPP 15.7 Mon 16:45 POT 81

Correlated states of moiré interlayer excitons in twisted transition metal dichalcogenide heterostructures — •Nils-Erik Schütte[1], Niclas Götting[1,2], Frederik Lohof[1,2], and Christopher Gies[1,2] — [1]Institute for Theoretical Physics, University of Bremen, Bremen — [2]Bremen Center for Computational Material Science, University of Bremen, Bremen

Stacking two transition metal dichalcogenide (TMD) monolayers on top of each other with a small relative twist yields a moiré pattern with a long lattice period. Quasiparticles perceive the resulting bandstructure modulation as a potential landscape, making it possible to consider moiré heterostructures as a realization of a Bose-Hubbard model in a semiconductor material.

We address the question in how far correlated states of moiré excitons can emerge and study their phase transition behavior in relation to the twist angle between both monolayers. Expanding on previous results [1], we discuss the effect of nearest-neighbor interaction that gives rise to a variety of different phases, such as inhomogeneous insulating and supersolid phases. Special attention is paid to the possibility of local atomic reconstructions that are now known to occur at small twist angles.

[1] Götting et al., Phys. Rev. B 105, 165419 (2022)

CPP 15.8 Mon 17:00 POT 81

Electronic structures of twisted bilayer graphene and tungsten diselenide investigated by transferable tight-binding-models — •Xiaoyu Liu, Stefan Blügel, and Hyun-Jung Kim — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Since the discovery of intrinsic unconventional superconductivity in the Moiré superlattice from bilayer graphene stacked with a small twist angle, a new venue so-called twistronics has opened. Beyond graphene, transition metal dichalcogenides as a class of two-dimensional (2D) materials have attracted much attention due to their interesting optical properties. With the growing interest in 2D layered materials, accurate models describing the band structure and electronic properties of twisted bilayer graphene and tungsten diselenide are highly desirable. Here, we provide sets of parameters for the transferable tight-binding (TB) model, based on the Slater-Koster (SK) scheme with the exponential scaling law for the interlayer and overlap integral parameters. The workflow, to obtain transferable TB model parameters, is automatized by introducing global optimization methods such as particle swarm optimization (PSO) and conformational space annealing (CSA) methods. The fitness of the parameter set is assessed not only by comparing with ab-initio band energies, but also with its orbital similarity. Accurately produced electronic structures of twisted bilayers graphene and tungsten diselenide provide a chance to research their unique electronic and optical attributes.
Hyun-Jung Kim acknowledges support by the AvH Foundation.

15 min. break

Invited Talk CPP 15.9 Mon 17:30 POT 81

Time-resolved optical spectroscopy of 3R-stacked MoS_2 — •Swarup Deb, Michael Kempf, Rico Schwartz, and Tobias Korn — Institute of Physics, Rostock University

Manipulation of in-plane rotational and out-of-plane stacking symmetry in engineered two-dimensional (2D) crystals has provided means to realize a variety of exotic phases in extremely thin structures. The emergence of out-of-plane ferroelectricity in rhombohedrally-stacked 2D materials, such as boron nitride and transition metal dichalcogenides (TMDs), is a recent addition to this, but so far, most research on rhombohedrally stacked (3R) TMDs focussed on bilayer units.

Here, we present a systematic study of low-temperature absorption, differential reflectivity, and Kerr rotation in 3R-stacked MoS_2 as a function of thickness, aiming to probe the effects of ferroelectricity and interlayer charge transfer on ground-state exciton properties, valley and photocarrier dynamics. We observe clear signatures of an energetic splitting of the A exciton, as well as valley and energy relaxation dynamics on a few-ps timescale.

CPP 15.10 Mon 18:00 POT 81

Constructing minimal tight-binding models for twisted TMDC bilayers — •Michael Winter, Dominik Benner, and Tim Wehling — I. Institute of Theoretical Physics, Universität Hamburg, Notkestraße 9-11, 22607 Hamburg, Germany

Transition metal dichalcogenides bilayers attract considerable attention within the last years due to the wide range of observable correlation effects, e.g. superconductivity, exciton condensation and therelike. One possible parameter to tune these phenomena is the twist angle between the two layers.

We study the electronic structure of twisted transition metal dichalcogenides from ab initio DFT calculations and subsequent Wannier construction on untwisted snapshots of commensurate structures. By choosing a subspace of only three Wannier orbitals per transition metal, we construct a minimal model for the description of twisted bilayers.

CPP 16: Nanostructures at Surfaces (joint session O/CPP)

Time: Monday 15:00–17:45 Location: GER 39

CPP 16.1 Mon 15:00 GER 39

Tailoring Stone-Wales transitions in Ti_2O_3 honeycombs with alkaline earth metals — •Martin Haller, Stefan Förster, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Institute of Physics, Von-Danckelmann-Platz 3, 06120 Halle, Germany

In 2013 the first 2D oxide quasicrystal (OQC) has been discovered in thin Ba-Ti-O films [1]. It shows a twelvefold diffraction pattern that is incompatible with lattice periodicity. In real space it can be described by squares, triangles and rhombus tiles. Just recently, the atomic structure has been solved [2,3]. The essence are Ti_nO_n ring structures with n = 4, 7 and 10. These evolve by Stone-Wales transitions from a pure honeycomb network [4]. The transformations are stabilized by alkaline earth metal ions and their associated dipole and can be controlled by the alkaline earth metal coverage. Here we investigate the basic steps of individual Stone-Wales transformations with LEED and STM for ultra-low coverages deposited onto a Ti_2O_3 honeycomb on a close-packed metal surface. The transformations to ring structures with n = 4, 5 and 7 are monitored and related to the formation of square and triangle tilings.

[1] S. Förster et al., Nature 502, 215 (2013)
[2] S. Schenk et al., Nat. Comm., accepted, (2022)
[3] E. Cockayne et al., Phys. Rev. B 93, 020101 (2016)
[4] S. Wang et al., Nanoscale 11, 2412 (2019)

CPP 16.2 Mon 15:15 GER 39

Formation of an extended quantum dot array driven and auto protected by an atom thick h-BN layer — •Joel Deyerling[1], Ignacio Piquero-Zulaica[1], Mustafa A. Ashoush[2], Knud Seufert[1], Mohammad A. Kher-Elden[2], Zakaria M. Abd El-Fattah[2], and Willi Auwärter[1] — [1]Physics Department E20, Technical University of Munich, James-Franck-Straße 1, D-85748 Garching, Germany — [2]Physics Department, Faculty of Science, Al-Azhar University, Nasr City, Cairo E-11884, Egypt

Fabricating nanoarchitectures to confine two dimensional nearly free electrons on crystalline surfaces by tip manipulation with a scanning tunneling microscope (STM) or by applying supramolecular chemistry principles yields diverse artificial electronic structures. These electronic states are prone to scattering by adsorbates making them extremely susceptible to the environment. Nonetheless, little attention has been given to their protection, e.g., by an inert overlayer.

Here, we show that a quasi-hexagonal CuS nanoporous network can be formed at the *h*-BN/Cu(111) interface by thermally-induced sulfur segregation from the Cu(111) bulk. The growth and structure is characterized by STM and X-ray photoemission spectroscopy. We demonstrate by employing STM and scanning tunneling spectroscopy that within the pores of the network the surface state of Cu(111) as well as the image potential states of *h*-BN/Cu(111) are confined, effectively creating arrays of quantum dots with well-defined sizes that are covered by an inert *h*-BN overlayer.

CPP 16.3 Mon 15:30 GER 39

First-principles investigation of doped borophene quantum dots as donor materials for solar cell applications — •Rachana Yogi, Vaishali Roondhe, and Alok Shukla — Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India

Because of fast-depleting fossil fuel reserves, there is an urgent need for harvesting alternative sources of energy. We present a first-principles atomistic study of borophene quantum dots (BQDs) B35 and B36 for their possible utilization in solar-cells. The pristine-BQDs are doped by C, N, and O atoms, and find that they have bowl-like structures in the ground state. The electronic and optical properties of pristine-BQDs, and doped-BQDs are investigated. The chemical potentials of several of these BQDs are slightly higher than that of popular solar-cell acceptor system PC71BM, they will act as electron donors in a PC71BM-based solar-cell. The calculated values of the open-circuit voltage corresponding to PC71BM and BQD-based device indicate efficient electron injection from the BQDs to PC71BM. O-doped B36-QD and B35-QD have the highest value of short-circuit current density attributed to their reduced HOMO-LUMO gap and high HOMO energy levels as compared to all other considered doped systems further enhancing the photoelectric properties. The power conversion efficiency of doped-BQDs exhibits significant improvement. The efficiency of O-doped B36-QD is maximum due to its high electron injection rate in PC71BM. Present calculations show that adding a foreign atom in BQD makes it a suitable candidate for high-performance solar-cells.

CPP 16.4 Mon 15:45 GER 39

Electrospray Depositions of a Spin-Crossover Active Iron(II) [2×2] Grid Complex on Ag(111) with Different Landing Energies — •Dennis Meier[1], Benedikt Schoof[1], Joachim Reichert[1], Nithin Surayadevara[2], Andreas Walz[1], Annette Huettig[1], Hartmut Schlichting[1], Mario Ruben[2], Anthoula C. Papageorgiou[1,3], and Johannes V. Barth[1] — [1]Technical University of Munich, Germany — [2]Karlsruhe Institute of Technology, Germany — [3]National and Kapodistrian University of Athens, Greece

Chiral spin-crossover (SCO) complexes are intriguing building blocks for innovative magneto-optical nanoarchitectures.[1] Such an Fe(II) [2×2] grid complex was deposited in ultra-high vacuum with electrospray controlled ion beam deposition (ES-CIBD)[2] on Ag(111) and investigated by scanning tunnelling microscopy. Low landing energy ($<$ 3 eV/z) resulted in clusters and single molecules. Higher landing energies ($>$ 3 eV/z) led to coordination bond cleavage and a rich variety of self-assembled surface networks forming from the grid fragments. Applying established on-surface synthesis methodology employing the possible constituents of these networks (ligands and Fe atoms) reproduced only a part of them. It is thus proposed that ES-CIBD provides an unexpected route to novel on-surface coordination network synthesis.

[1] N. Suryadevara et al. *Chem. Eur. J.* 2021, **27**, 15172.
[2] A. Walz, K. Stoiber, A. Huettig, H. Schlichting, J. V. Barth, *Anal. Chem.* 2022, **94**, 7767.

CPP 16.5 Mon 16:00 GER 39

Giant confinement of surface electrons in a two-dimensional metal-organic porous network — •Lu Lyu[1], Tobias Eul[1], Wei Yao[1], Zakaria M. Abd El-Fattah[2], Mostafa Ashoush[2], Ignacio Piquero-Zulaica[3], Johannes V. Barth[3], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,4] — [1]Department of Physics, University of Kaiserslautern, Germany. — [2]Physics Department, Faculty of Science, Al-Azhar University, Egypt. — [3]Physics Department E20, Technical University of Munich, Germany — [4]Institute of Physics, Johannes Gutenberg University Mainz, Germany.

Two-dimensional metal-organic porous networks (2D-MOPNs) are highly flexible nano-architectures for exploring the quantum confinement of surface electrons on noble metals. So far, 2D-MOPNs have been predominantly studied for the confinement of occupied Shockley-type surface states (SS). In contrast, the confinement of excited surface states, such as image potential states (IPSs), remains elusive. In this work, we apply two-photon photoemission to investigate the band dispersion of the first image-potential state (n = 1 IPS) in a Cu-T4PT nanoporous network on Cu(111). We find the formation of a Bloch-like band structure with a substantially increased effective band mass of the IPS ($>$ 150 %). In contrast, the effective band mass of the SS remains almost unchanged ($<$ 3%). This band renormalization of the IPS can be attributed to the spatial distribution of its charge density perpendicular to the surface, which reveals the highest density at the vertical adsorption position of the T4PT backbone. This coincidence is responsible for the giant confinement.

CPP 16.6 Mon 16:15 GER 39

Modification of Single-Layer Organometallic Networks: from Ag-Bridged to Cu-Bridged Alkynyl Metal-Alkynyl Linkages on Ag(111) Surfaces — •Wenchao Zhao, Felix Haag, Ignacio Piquero-Zulaica, Yi-Qi Zhang, Francesco Allegretti, Biao Yang, and Johannes V Barth — Physics Department E20, Technical University of Munich, 85748 Garching, Germany

The metal-exchange reaction, is of importance for the advanced preparation of functional metal-organic frameworks for various applications[1]. Notably, building two-dimensional organometallic networks (OMNs), can provide versatile nanoarchitectures for potential application in nanodevice[2,3]. Although various OMNs have been constructed with molecular building blocks by abstracting surface metal atoms, the degree of success is often individual and substrate-dependent. Thus metal-exchange reactions hold promise for multiple production by modification and functionalization of OMN templates. Here, we demonstrate the modification of a single-layer OMN by metal-exchange reaction. By introducing external Cu atoms into the alkynyl-Ag OMN[3], we successfully synthesized in situ a highly ordered alkynyl-Cu OMN on a Ag(111) surface. While maintaining a similar lattice periodicity and pore morphology, it possesses higher thermal stability, guaranteeing higher robustness for possible applications. Reference. 1. M.-M. Xu et al., Coord. Chem. Rev. 2020, 421, 213421. 2. D. Ecija et al., Acc. Chem. Res. 2018, 51, 365-375. 3. Y.-Q. Zhang et al., J. Am. Chem. Soc. 2019, 141, 5087-5091

CPP 16.7 Mon 16:30 GER 39

Structure Formation in Ceramic Thin Films with Hybrid Molecular Dynamics — •Nydia Roxana Varela Rosales and Michael Engel — Institute for Multiscale Simulation, University of Erlangen-Nürnberg, Cauerstraße 3, 91058 Erlangen, Germany

How can we model and predict ceramic thin films? Highest accuracy is achieved with ab-initio quantum mechanical methods. But these methods are not suitable for large systems including their phase transformations. Atomistic modeling with molecular dynamics and Monte Carlo simulations reaches large system sizes but require sophisticated tailored interaction potentials. Here, we develop and apply a coarse-grained simulation method for structure formation in thin films. Our method considers the chemical bond network of the ceramics explicitly to simplify the complexity of the simulation and to reach high simulation speeds and large system sizes. Of particular interest are (quasi-)crystalline ceramic thin films recently discovered in experiments of (Ba/Sr)-Ti-O perovskites. Solely by considering the extrinsic topology of the tiles and utilizing a harmonic interaction potential, we reproduce the appearance of approximants of the dodecagonal quasicrystals, which was also predicted by ab-initio simulations. Our work highlights the role of bond network topology in understanding complex thin film structures without a need for reliance on quantum simulation methods.

CPP 16.8 Mon 16:45 GER 39

A Holistic Characterisation of Bi Thin Films on Au(111) — •Pablo Vezzoni Vicente[1], Tobias Weiss[1], Marc Gonzalez-Cuixart[4], Dennis Meier[1], Benedikt Klein[2], David Duncan[2], Ezequiel Tosi[3], Paolo Lacovig[3], Silvano Lizzit[3], Johannes Barth[1], Peter Feulner[1], and Francesco Allegretti[1] — [1]Physics Department E20, Technische Universität München, Germany — [2]2I09 beamline, Diamond Light Source, United Kingdom — [3]3SuperESCA beamline, Elettra Synchrotron, Italy — [4]4IMDEA Nanociencia, Spain

We present a comprehensive analysis of the long-range ordered, coverage-dependent phases of Bi epitaxially grown on a Au(111) surface in UHV, from the sub-monolayer $(\sqrt{37} \times \sqrt{37})R25.3^\circ$ Kagome lattice up to few-layer Bi(110) thin films. Particular focus is devoted to the sub-monolayer, high-coverage $(p \times \sqrt{3})$ phase, paving the way to its use as a buffer layer for epitaxial growth with tunable geometry and low electronic interaction.

Our work clarifies and expands the current literature reports, specifically on the complex $(p \times \sqrt{3})$ phase. The wide range of analysis techniques used, including Low-Energy Electron Diffraction (LEED), Photo-Electron Spectroscopy (XPS, UPS), Temperature Programmed Desorption (TPD), Scanning Tunneling Microscopy and Spectroscopy (STM, STS), and X-ray Standing Waves (XSW), yields an unprecedented understanding of the system's structural and electronic properties.

CPP 16.9 Mon 17:00 GER 39

Analytical electron microscopy of nanostructured vanadium dioxide — •Vlastimil Křápek[1], Jan Krpenský[1,2], Michal Horák[1], Katarína Rovenská[1], Peter Kepič[1], Tomáš Šikola[1], Filip Ligmajer[1], and Andrea Konečná[1] — [1]Brno University of Technology, Czechia — [2]CIC nanoGUNE, San Sebastián, Spain

Vanadium dioxide (VO_2) is a phase-changing material exhibiting temperature-induced metal-insulator transition (MIT) around 340 K. A rather low transition temperature makes VO_2 a suitable material for active nanophotonics, e.g., switchable optical metasurfaces. Such applications require nanostructuring of VO_2 thin films. Here we study the possibility to employ focused ion beam (FIB) milling for the nanofabrication and its impact on the properties of resulting nanostructures.

Taking the VO_2 thin film with experimentally verified MIT, we utilized FIB milling with Ga ions to fabricate V-shaped lamella of the thickness between 0 and 250 nm, which was subsequently transferred onto a heating chip for transmission electron microscopy and analyzed with analytical electron microscopy: high-resolution imaging, energy-dispersive X-ray spectroscopy, and temperature-dependent electron energy loss spectroscopy. We observed a porous character of the pristine material, a coexistence of several crystal structures, negligible contamination with Ga ions, and a variation of stoichiometry with the thickness of the lamella, with the thinnest parts composed of VO and V_2O_3.

CPP 16.10 Mon 17:15 GER 39

Tuning Nanoporous Au Film Formation via High Voltage Electrolysis — •Evelyn Artmann[1], Lukas Forschner[1], Konstantin M. Schüttler[2], Mohammad Al-Shakran[1], Timo Jacob[1], and Albert K. Engstfeld[1] — [1]Institute of Electrochemistry, University of Ulm, Germany — [2]Institute of Surface Chemistry and Catalysis, University of Ulm, Germany

Nanoporous Au (NPG) films have different properties compared to the bulk material, which opens up new areas of application, such as (electro)catalysis. Usually, NPG films are prepared by dealloying. One disadvantage of this method is that residues of the precursor alloy guest metal can remain in the resulting NPG film, which can have a decisive influence on the electrocatalytic activity of the NPG film.

In this work we report on the preparation of NPG films by high voltage electrolysis (Chem. Phys. Chem., 22 (2021) 2429). In this process, a Au oxide film is first formed on the Au substrate by applying a high positive voltage (between 100 and 540 V), which can subsequently be reduced to NPG. The Au oxide as well as NPG films were characterized by electrochemical methods, as well as (cross-section) SEM and XPS measurements.

Possibilities to selectively modify the resulting NPG films by tuning experimental parameters such as the applied voltage, and electrolyte temperature during HV electrolysis, or the electrolysis time, were systematically investigated. The influence of the reduction method (electrochemical or by H2O2) on the final film structure is discussed.

CPP 16.11 Mon 17:30 GER 39

Evolution of the Si-Au alloy: from the gold (110) substrate to silicon nanoribbons — •Ekaterina Tikhodeeva[1], María E Dávila[2], Paola De Padova[3], Gay Le Lay[4], Marina Baidakova[5], Evgeniya Lobanova[5], Jaime Sanchez-Barriga[6], Dmitrii Smirnov[6], and Manuel Izquierdo[1] — [1]European XFEL, Schenefeld, Germany — [2]CSIC, Madrid, Spain — [3]Consiglio Nazionale delle Ricerche, Rome, Italy — [4]Aix-Marseille Université, Marseille, France — [5]Saint Petersburg, Russia — [6]Helmholtz-Zentrum Berlin, Berlin, Germany

The development of the Si-Au alloy was investigated on the path from the gold single crystal surface to silicon nanoribbons (SiNR). Si sub-monolayers were deposited on the missing row reconstructed Au(110) substrate. At various stages of evaporation, low-energy electron diffraction (LEED) patterns were recorded to refine the surface geometry. The arrangement of the Si atoms has been correlated with the missing row orientation. The recovery of the Au(1x1) reconstruction, as well as the gradual transition from surface alloy to SiNRs were explored. In parallel with LEED, photoelectron spectroscopy was used to clarify the atom distribution. The profiles of the Au 4f and Si 2p core levels were deconvoluted and analyzed at all stages of Si deposition. The appearance of a new low kinetic energy component was noticed in the Au 4f spectra. It is related to the Si-Au bond and indicates a strong interaction between them. The Si core levels exhibit up to three components corresponding to the different chemical environments.

CPP 17: Poster Session I

Topics: Focus: Self-Assembly of Plasmonic Nanostructures (1-4); Molecular Electronics and Excited State Properties (5-10); Organic Electronics and Photovoltaics (11-30); Hybrid and Perovskite Photovoltaics (31-44); Charged Soft Matter, Polyelectrolytes and Ionic Liquids (45-48); Interfaces and Thin Films (49-57), 2D Materials (58-60).

Time: Monday 18:00–20:00 Location: P3

CPP 17.1 Mon 18:00 P3

Plasmonic behaviour of surface modifications of γAlOOH nanoparticles and their effect on the particles Hamaker constant — •Dorothee Silbernagl[1], Mateusz Dudziak[1], Anna Maria Manzoni[1], and Heinz Sturm[1,2] — [1]Bundesanstalt für Materialforschung und -prüfung, Unter Den Eichen 87, 12205, Berlin, Germany — [2]Institute for Machine Tools and Factory Operations (IWF), TU Berlin, Pascalstr. 8-9, 10587 Berlin, Germany

Boehmite (γAlOOH) nanoparticles (BNP, particle size appr. 14nm) are known for their extremely low Hamaker constant A, which results in low interparticle van der Waals forces. However, surface modified BNPs (modifications are acidic acid BNPA, lactic acid BNPL and stearic acid BNPS) exhibit a gradually increased Hamaker constant A and therefore increased interparticle van der Waals forces. This was measured by atomic force microscopy force distance curves (AFM FDC). For this experiment an unmodified BNP agglomerate of approximately 50um diameter was attached to an AFM cantilever and measured against pressed BNPs without and with different surface modifications. This set-up provides a sphere/plane geometry, necessary to calculate the Hamaker constant A of each material pairing from the FDCs attractive regime. Electron energy loss spectroscopy (EELS) measurements in the low energy region (up to 80eV) of unmodified and surface modified BNPs were performed to understand the origin of the increased van der Waals forces. As a result, additional plasmon bands were found in the region below 10eV for surface modified BNPs, which contribute to the attractive forces between particles.

CPP 17.2 Mon 18:00 P3

Liquid phase (S)TEM of DNA origami gold nanoparticle hybrids — •A. Ong[1], D. Pohl[1], T.K. Jeong[2,3], A. Heerwig[2,3], M. Mertig[2,3], and B. Rellinghaus[1] — [1]Dresden Center for Nanoanalysis (DCN), cfaed, TU Dresden, Germany. — [2]Physical Chemistry, TU Dresden, Germany — [3]Kurt-Schwabe-Institut für Mess- und Sensortechnik Meinsberg e.V., Germany

DNA origami pads with site-specific patterns of ssDNA are flexible molecular templates for gold nanoparticles to self-assemble into functional supracolloidal structures [1]. The structure-property relation of supracolloidal structures play a significant role in constructing novel materials with desired properties for application in devices [2]. However, this relation has not been adequately understood. The study focuses on investigating the self-assembly and kinetic processes in supracolloidal structures using (scanning) transmission electron microscopy [(S)TEM] both in vacuum and in the liquid phase. Images of gold nanoparticles attached to DNA origami were acquired under vacuum and in-situ in the liquid phase, highlighting the possibility of real-time visualizations at the nanometer scale in different environments. The measured distances between gold nanoparticles in liquid confirm the intended templating mechanism. Financial support by DFG through RTG 2767 and by the EU Horizon 2020 Research & Innovation Programme grant agreement no. 964248 is gratefully acknowledged.

[1] J. Zessin et al. Nano Lett. (2017)17, 5163.

[2] T. Woehl, ACS Nano (2019) 13, 12272.

CPP 17.3 Mon 18:00 P3

Probing photoluminescent polymers using plasmonic self-assembly — •Onima Bisht[1,3], Sezer Seçkin[1], and Tobias König[1,2] — [1]Leibniz-Institut für Polymerforschung e.V., Hohe Straße 6, 01069 Dresden, Germany — [2]Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, 01062 Dresden, Germany — [3]Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, 110016, India

Surface Enhanced Raman Spectroscopy (SERS) is an advantageous and indispensable technique for detection and sensing applications. Although SERS substrates have been fabricated using several top-down approaches, these methods are limited by scalability, uniformity, and high instrumentation costs. Recent developments in template-assisted self-assembly (TASA) techniques have facilitated us to fabricate low-cost, scalable, and uniform gratings consisting of plasmonic nanoparticle chains.[König et al., Adv. Funct. Mater. 2021, 2105054] With the support of the finite-difference time-domain (FDTD) method, we have rationally designed the colloidal grating to benefit from the coherent interaction between Rayleigh anomalies and various plasmon modes. We will combine these modes with the quantum emitter, which we used previously as an efficient gain component for optoelectronic devices. [König et al., Adv. Optical Mater. 2020, 2001280] Finally, we use this overlap of the plasmonic modes with the photoluminescence of the emitters for nonlinear effects such as lasing, strong coupling, and ultra-high SERS sensitivity.

CPP 17.4 Mon 18:00 P3

Influence of thermal effects on a combinatorial plasmonic nanostructure for bio-detection — •Tianfu Guan[1], Suzhe Liang[1], Yusuf Bulut[1,2], Kristian Reck[3], Matthias Schwartzkopf[2], Jonas Drewes[3], Thomas Strunskus[3], Franz Faupel Faupel[3], Stephan V. Roth[2,4], and Peter Müller-Buschbaum[1,5] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]DESY, 22607 Hamburg, Germany — [3]CAU, Chair for Multicomponent Materials, Faculty of Engineering, 24143 Kiel, Germany — [4]Department of Fiber and Polymer Technology, KTH, SE-100 44 Stockholm, Sweden — [5]MLZ, TUM, 85748 Garching, Germany

In recent decades, Au nanoparticles (NPs) have been utilized in a wide range of sensor applications, such as photodetection, bio-detection, and thermal-detection, because of their unique optical and chemical properties. Among the optical sensors, surface-enhanced Raman spectroscopy (SERS) has attracted extensive attention being used in the identification of unknown substances in analytical chemistry. In this work, we investigate in situ sputter deposition of Ag on highly ordered Au NPs substrates as probed by grazing incidence small angle X-ray scattering (GISAXS). In addition, we explore the effect of temperature on the silver growth kinetics on different sizes of Au NPs substrates. Furthermore, by correlating the growth steps of the composite Au/Ag nanostructures with their SERS performance, we obtain the plasmonic hot spot performance corresponding to the combined nanostructure.

CPP 17.5 Mon 18:00 P3

Understanding the Double Doping of Organic Semiconductors Via State Energy Renormalization upon Charging — •Ross Warren[1], Eunkyung Cho[2], Hong Li[2], Jean-Luc Bredas[2], and Norbert Koch[1,3] — [1]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Department of Chemistry and Biochemistry, The University of Arizona, Tucson, Arizona 85721-0088, United States — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany

The double ionisation of dopants is a recent experimental observation that allows the doping efficiency to rise above 100%. This is exciting because high conductivities can be achieved with fewer dopant molecules, meaning less disruption to the resulting film's microstructure. However, the current models of doped organic semiconductors based on Fermi-Dirac statistics fail to explain the double ionization of dopants and also the analogous situation of bipolaron formation on a host polymer. Here, we address this shortcoming by considering the renormalization of the state energies upon electron transfer between host and p-dopant. We vary the model parameters - the reorganization energy and evolutions of ionization energies and electron affinities upon charging - and plot the fractions of doubly ionized, singly ionized, and neutral species. We find good agreement with experiment. Finally, we suggest that the state energy renormalization upon charging is the key parameter to be minimized for double ionization of dopants or maximized to avoid formation of bipolarons on the host.

CPP 17.6 Mon 18:00 P3

Temperature Dependent Photoluminescence of β-Phase Zinc Phthalocyanine Single Crystals — •Kilian Strauss[1], Lisa Schraut-May[1], Sebastian Hammer[1,2], Kilian Frank[3], Bert Nickel[3], and Jens Pflaum[1] — [1]Experimental Physics VI, Julius-Maximilians-Universität of Würzburg — [2]Department of Physics, Ludwig Maximilian University, Munich — [3]Departments of Physics and Chemistry, McGill University, Montreal, Canada

The photophysical properties of organic crystals are strongly dependent on the interactions between the comprising molecules. We chose zinc phthalocyanine (ZnPc) in its crystallographic β-phase as a model system to investigate the excitonic coupling as a function of crystallographic direction. For this purpose, we performed polarization dependent photoluminescence (PL) measurements from 5 K to 300 K on needle-shaped single crystals grown by horizontal vapour deposition. A gradual optical transition from a J- to H-aggregate like behavior occurs on cooling down to 100 K. Upon further cooling, we find the emergence of superradiant luminescence typical for exciton delocalization in J-aggreagtes. This optical transition is induced by an anisotropic thermal compression of the crystal lattice.
We thank the Bavarian Research Network SolTech for financial support.

CPP 17.7 Mon 18:00 P3

On the Parametrization of Exciton-Phonon Coupling Matrix Elements by Ab Initio Methods — •Maximilian Franz Xaver Dorfner and Frank Ortmann — Department of Chemistry, Technische Universität München, 85748 Garching b. München, Germany

The accurate description of optical or transport properties of organic semiconductors, such as small molecules or polymers requires, besides the electronic degrees of freedom, also the incorporation of the nuclear motion into the theoretical treatment. This is because in these materials the electrons and the core movement are significantly coupled to each other.

This interaction co-determines macroscopic observables, like absorption cross-sections, charge carrier mobilities, or electronic relaxation time-scales. Close to the equilibrium configuration, the interplay of the electronic degrees of freedom and the nuclei can be cast into the form of a Holstein-Peierls model. In this representation, the interaction is characterized by a set of coupling constants, which are typical for a given molecule and dictate behavior in a range around the equilibrium configuration.

Here we present a novel scheme and an implementation for the computation of these effective coupling constants based on the CP2K software package. We benchmark our implementation for a number of molecules and study their non-radiative electronic relaxation behavior by the use of a matrix product state approach.

CPP 17.8 Mon 18:00 P3

Unraveling Structural Dynamics in Excimer Formation Using Ultrafast Electron Diffraction — •Sebastian Hammer[1], Laurenz Kremeyer[1], Tristan Britt[1], Maximilian Rödel[2], Syed Ali Hassan[1], Jens Pflaum[2,3], and Bradley Siwick[1] — [1]Departments for Physics and Chemistry, McGill University, Montreal, QC H3A 2K6, Canada — [2]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [3]Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

Excimer formation, *i.e.* the formation of an excited dimer state which is accompanied by structural deformations in the local inter-molecular geometry, is a common phenomena in molecular solids and crucially determines the opto-electronic properties of the material. While the process is understood well on a theoretical level [1], direct observational evidence of the underlying structural dynamics are experimentally challenging.

In recent years, the technique of ultrafast electron diffraction (UED) has proven to be capable of unraveling the structural dynamics of molecular single crystals after photo-excitation [2]. Using the prototypical excimer system zinc-phthalocyanine in its crystallographic α-phase [3], we show that UED experiments on polycrystalline thins-films can disclose the structural dynamics accompanying excimer formation. We gratefully acknowledge funding from the DFG (Project 490894053).

[1] Bialas et al. *J. Chem. Phys. C.* **126** 4067-4081 (2022)

[2] Gao et al. *Nature.* **496** 343-346 (2013)

[3] Hammer et al., *Mater. Horiz.*. (2022)

CPP 17.9 Mon 18:00 P3

Influence of Ligands and Linker on the Optoelectronic Properties of Phenazine-based Iron Spin-Crossover Complexes — •Lydia Ploss[1], Florian Daumann[2], Konstantin Schötz[1], Gerald Hörner[2], Birgit Weber[2], and Anna Köhler[1,3] — [1]Experimental Physics II, University of Bayreuth — [2]Anorganische Chemie IV, University of Bayreuth — [3]Bayreuth Institute of Macromolecular Research, University of Bayreuth

Spin-crossover (SCO) complexes are a class of materials - typically organo-metallic complexes - whose electronic ground state can be switched between a high spin (HS) and a low spin (LS) state by external stimuli, e.g., by varying the temperature. This possibility renders them promising candidates for applications such as molecular switches or sensors.

An easy way to read out sensors is, e.g., by using photoluminescence (PL) spectroscopy. Recently, an iron-based SCO complex was found that shows PL in both spin states.[1] This is remarkable since most SCO complexes show PL in only one of the two spin states or are not luminescent at all. To understand what defines the optical properties of such compounds, we systematically vary ligands and linker molecules of the complexes and investigate their influence on the optical properties of the resulting complexes, using absorption and temperature-dependent PL spectroscopy.

[1] Lochenie et al., J. Am. Chem. Soc. 2018, 140, 2, 700-709

CPP 17.10 Mon 18:00 P3

Multichromophore Macrocycles of Perylene Bisimide Dyes as Fluorescent OLED Emitters — •Theodor Kaiser[1], Björn Ewald[1], Ulrich Müller[1], Peter Spest[2], Mathhias Stolte[2], Frank Würthner[2], and Jens Pflaum[1] — [1]Experimental Physics VI, University of Würzburg — [2]Institut für Organische Chemie and Center for Nanosystems Chemistry, University of Würzburg

While fluorescent organic emitters exhibit an efficient and bright singlet decay their efficiency in Organic Light Emitting Diodes (OLEDs) is limited by the lifetime and non-radiative loss pathway of triplet dark states. Therefore OLED applications are mainly based on phosphorescent emitters harvesting triplet excitons for light emission. In order to increase the efficiency of fluorescent OLEDs we present a novel approach for the chemical design of fluorescent emitters based on multichromophore macrocycles of perylene bisimide dyes (PBIs). By linking individual PBI chromophores in macrocyclic architectures, biexcitonic coupling can lead to an efficient transformation of triplet dark states by processes like triplet-triplet annihilation (TTA). This allows for an efficient bright electrical operation in OLED devices as the lifetime of dark states is drastically reduced. As recently reported by our groups trimeric perylene bisimides can even produce non-classical electrically driven single photon emission at room temperature [1], which has so far only been reported for phosphorescent emitters. Therefore these emitters offer new options for the application of strictly fluorescent materials in classical and non-classical OLED devices.

[1] Ulrich Müller et al.,Adv. Optical Mater 2022, 10, 2200234.

CPP 17.11 Mon 18:00 P3

Investigation of Metal–Insulator Transitions in Organic Field-Effect Transistors of an n-Type Organic Semiconductor — •Paul Schlachter[1], Maximilian Frank[1], Matthias Stolte[2], Frank Würthner[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]Institut für Organische Chemie and Center for Nanosystems Chemistry, University of Würzburg, 97074 Würzburg — [3]ZAE Bayern, 97074 Würzburg

Metal-insulator transitions in organic materials offer many exciting applications and are therefore gaining increasing scientific as well as technological interest. In this work, we aim to investigate electronic field-effect-induced phase transitions (semiconductor → conductor → insulator) in organic single crystals (especially Cl_2NDI [1]) of high electron mobility. The long-range order of their molecular entities in combination with a preferred (001) gliding plane geometry provides the pre-condition of a nearly defect-free interface for studying quasi-two-dimensional electron gas formations. For this purpose, we use an electrolyte as a top gate in addition to a dielectric conventional back gate. By simultaneously varying the bottom and top gate voltages, respectively, we aim to control the charge carrier density and thereby to gain deeper insights into Mott physics. First results on these efforts will be presented and evaluated with respect to the possible implementation in Mott field-effect transistors.

[1] Tao He et al., Nat. Commun. 2015, 6, 5954

CPP 17.12 Mon 18:00 P3

On the orientation mechanism of non-polar dyes in light-emitting guest-host systems — •Binh-Minh Nguyen, Markus

Schmid, Johann Kirsch, and Wolfgang Brütting — Experimental Physics IV, Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

After many years of development, OLEDs have continuously been optimized to reach higher efficiency, for which the horizontal orientation of the emitter molecules is one of the dominant factors [1]. For the purpose of studying intrinsic orientation without electrostatic interaction, our work considers non-polar dyes, namely TTPA, BSBCz, DIP and DBP. While the emitter orientation has been studied in neat film as a basic approach, their behavior in guest-host systems has not been studied widely. In this work we focus on the correlation between emitter concentration and its orientation. With the results from experimental and simulation study, we also discuss the possible orientation mechanism of emitter molecules on the substrate surface in terms of molecular structure, possibility to form crystallites and the effective glass transition temperature of the guest-host system. We observe that isotropic structure of the emitter as well as the crystallized and aggregated molecules are not favorable for horizontal orientation. However, molecules having a rod-like structure have the tendency to arrange horizontally to the substrate. These results contribute to a further understanding of orientation of non-polar emitter molecules.

[1] Brütting et. al, Physical Review Applied, 2017, 8(3), 037001.

CPP 17.13 Mon 18:00 P3

Self-heating in OLED Lighting — •Anton Kirch[1,2], Axel Fischer[1], Matthias Liero[3], Jürgen Fuhrmann[3], Annegret Glitzky[3], Ludvig Edman[2], and Sebastian Reineke[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), TU Dresden, Germany — [2]Department of Physics, Umeå University, Sweden — [3]Weierstrass Institute Berlin, Germany

For bright area light sources, such as OLED lighting tiles, the electric resistivity of transparent electrodes induces a non-uniform current distribution within the device. At high driving currents, the interaction between conductivity, heat, and power dissipation results in a positive electrothermal feedback loop, which drastically exacerbates inhomogeneities in local device temperature and luminance.

Such nonlinear behavior induces unprecedented electrothermal effects that compromise the performance of bright area light sources. In this contribution, we present how Joule self-heating squeezes temperature and current into a tiny device region, while the remainder of the active area decreases in luminance (Switch-back effect) [1]. We further introduce how the dimension of the active area governs the current-voltage characteristics of the OLED and how two and even three stable operating branches develop (tristability) that can promote destructive incidences [2].

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CPP 17.14 Mon 18:00 P3

Organic Photoconductors based on Rubrene Thin-Films — •Jonas Schroeder, Rishabh Rishabh, Johannes Benduhn, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Nöthnitzer Str. 61, 01187 Dresden, Germany

Thin films of organic semiconductors possess huge potential for large-scale industrial applications. However, the limited possibilities of crystal growth directly on the substrates often restrict device concepts but also achievable device performance. Here, we use vacuum-deposited rubrene in combination with a thermal post-treatment to fabricate different morphologies of polycrystalline thin films. To take advantage of the high in-plane mobility ($3\,\mathrm{cm^2\,V^{-1}\,s^{-1}}$) of the well-known orthorhombic rubrene phase in light detection applications, we employ photoconductive detectors in which the contacts are placed laterally on the sides of the active material. This allows for decoupling of the filtering of the incident light from the channel geometry and a photocurrent gain due to the natural imbalance of electron and hole mobilities in organic semiconductors. We show performance benchmarks of prototypical photoconductive organic photodetectors and relate these to the optical and electrical properties of the used rubrene thin films.

CPP 17.15 Mon 18:00 P3

Optimizing narrowband OPDs for wavelength range from 700 nm to 1100 nm — •Fred Kretschmer, Louis Conrad Winkler, Jakob Wolansky, Johannes Benduhn, and Karl Leo — Technische Universität Dresden, Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics (IAP), Dresden, Germany

In recent years, organic photodetectors have attracted particular interest, due to their advantageous properties, such as cheap manufacturing costs and high performance, compared to inorganic devices. Particularly important is the narrowband photo-response, which enables the detection of small wavelength ranges, making optical filters obsolete and allowing miniature detector compositions. Narrowband spectroscopic sensors are an integral part of modern society, for example, in food quality monitoring, signal communication, or medical imaging.

In this contribution, microcavity-enhanced organic photodetectors in the visible and near-infrared wavelength range are investigated. For these devices, the active and transport layer thickness are varied and analysed for the donor material Rubrene and Spiro-MeO-TPD. Therefore, performance parameters such as the external quantum efficiency, the specific detectivity, the dark current, the response speed, and parasitic side effects are investigated and examined, leading to concrete device guidelines which can increase the performance of narrowband organic photodetectors. In a next step, we are planning to complement these detectors with infrared light-emitting diodes for a fully organic, spectroscopic sensing system.

CPP 17.16 Mon 18:00 P3

Humidity Stable Thermoelectric Hybrid Materials for A Self-Powered Sensing System — •Suo Tu[1], Ting Tian[1], Tianxiao Xiao[1], Shanshan Yin[1], Julian Heger[1], Guangjiu Pan[1], Shujin Hou[2], Aliaksandr Bandarenka[2], Matthias Schwartzkopf[3], Stephan Roth[3], and Peter Müller-Buschbaum[1,4] — [1]Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, 85748 Garching — [2]Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Physik der Energiewandlung und -speicherung, 85748 Garching — [3]DESY, 22607 Hamburg — [4]MLZ, TUM, 85748 Garching

Highly sensitive and humidity-resistive detection of the most common physical stimuli is of primary importance for practical application in a real-time monitoring. Here, we report a simple yet effective strategy to achieve a highly humidity-stable hybrid composite that enables simultaneous and accurate pressure and temperature sensing in a single sensor. The improved electronic performance was due to the enhanced planarity of PEDOT and charge transfer between PEDOT:PSS and multi-walled carbon nanotubes (MWCNT) by strong π-π interaction. The preferred electronic pathway induced by robust morphology in the hybrid composite is responsible for the high humidity stability. These observations have been recognized by Grazing-incidence wide/small-angle X-ray scattering (GIWAXS/GISAXS), Raman, FTIR, and electrochemical impedance spectroscopy (EIS).

CPP 17.17 Mon 18:00 P3

New insights into the P3HT:PCBM bulk-heterojunction — •Shahidul Alam[1], Christopher E. Petoukhoff[1], Haya Aldosary[1], Xinyu Jiang[2], Tomáš Váry[3], Wejdan Althobaiti[1], Sandra P. Gonzalez Lopez[1], Wejdan Alsufyani[1], Peter Müller-Buschbaum[2], Vojtech Nádaždy[4], Harald Hoppe[5], and Frédéric Laquai[1] — [1]KAUST Solar Center (KSC), Kingdom of Saudi Arabia — [2]TU Munich, Germany — [3]STU Bratislava,Slovak Republic — [4]Slovak Academy of Sciences, Bratislava, Slovak Republic — [5]FSU Jena, Germany

Here, we studied the influence of thermal annealing on blends of well-known regio-random and regio-regular P3HT conjugated polymers and fullerene derivative [6,6]-phenyl-C60-butyric acid methyl ester (PC60BM). Several advanced microscopic and spectroscopic techniques were applied to investigate the thermal annealing effects on the structural, morphological, and energetic states, e.g., grazing-incidence wide-angle x-ray scattering, polarized light microscopy, hyperspectral photoluminescence spectroscopy, and photo-deflection spectroscopy. Furthermore, the blends' density of states (DOS) distribution was studied using energy resolved-electrochemical impedance spectroscopy. Coupled transfer matrix methods and drift-diffusion simulations were employed to see the impact of DOS on the solar cells' device parameters.

CPP 17.18 Mon 18:00 P3

Crystal Orientation and Surface Morphology in Thin Films of Poly-[3-(6-trifluorohexyl)thiophene] on Silicon and Graphene — •Alexander Much[1], Robert Kahl[1], Florian Meichsner[2], Mukundan Thelakkat[2], Thomas Thurn-Albrecht[1], and Oleksandr Dolynchuk[1] — [1]Experimental Polymer Physics, Martin Luther University Halle-Wittenberg — [2]Applied Functional Polymers, University of Bayreuth

Semiconducting polymers gained much interest for use in electronic devices due to their easy processing from solution and mechanical flexibility. To improve the efficiency of organic electronic devices, it is crucial to understand and control the crystal orientation in thin films.

As recently found in films of poly-(3-hexylthiophene) (P3HT) on graphene, the interfaces to vacuum and graphene induce edge-on and face-on orientation, respectively [1]. We propose to influence the crystal orientation in polythiophenes by increasing the polarity of the end group of the side chains. Thereby, melt-crystallized thin films of poly-[3-(6-trifluorohexyl)thiophene] (P3CF3HT) studied by GIWAXS showed an increased and thickness-dependent tendency to face-on orientation not only on graphene, but also on silicon, which is inactive for P3HT. Furthermore, the film surface morphology probed by AFM strongly depends on the crystal orientation and the substrate. Our results validate the approach and open a pathway to control molecular orientation in polythiophenes.

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CPP 17.19 Mon 18:00 P3

Influence of amphiphilic additives on P3HT:PC60BM organic solar cells — •Jose Prince Madalaimuthu[1,2], Zhuo Xu[1,2], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstr. 10, D-07743 Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, D-07743 Jena, Germany

The mechanical stability of the layer stack is a significant barrier to the continued functioning of flexible OPVs. Delamination processes have the potential to significantly reduce photovoltaic performance. High-crystallinity polymers retain blend morphologies for a long time but yield brittle thin films. Amorphous polymers produce more flexible films but have less morphological stability. Device performance is associated with high crystallinity and superior charge carrier mobility. Furthermore, the elasticity required for mechanical stability is often improved with more amorphous polymers. This seems to split the necessary material characteristics in two. The objectives of the investigations are to improve mechanical resilience by lowering the tensile modulus and reducing crystallization by introducing tiny amounts of amphiphilic plasticizers. The effect of amphiphilic small molecule additions in donor-acceptor blends was investigated for toluene sulfonic acid (TSA) and then with a series of perylenes with systematically varying amphiphilicity. Enhancing the device's performance and long-term stability illustrates that the active layer's morphology can be regulated by the presence of amphiphilic additives.

CPP 17.20 Mon 18:00 P3

Enhanced air stability of green-solvent polymer solar cells with green-fluorescent polymer EH-P — •Zerui Li[1], Sergei Vagin[2], Kun Sun[1], Morgan Le Dû[1], Manuel A. Reus[1], and Peter Müller-Buschbaum[1,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, James-Franck-Str. 1, 85748 Garching, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Department of Chemistry, Chair of Macromolecular Chemistry, James-Franck-Str. 1, 85748 Garching, Germany — [3]Technical University of Munich, MLZ, Lichtenbergstr. 1, 85748 Garching, Germany

The rapid development of materials has promoted that the efficiency of polymer solar cells (PSCs) reached over 20%, which is highly close to the application requirement. While the relative poor stability of PSCs slows down their commercial progress. Nowadays the research of stability in nitrogen or vacuum recieved much attention, while the inevitable contact of air would also cause undesirable effect on the device performance. Here, we select a green-solvent based material system PBDB-TF-T1:BTP-4F-12 as research model. Firstly the degradation of solar cells in air was observed and the mechanism was investigated. Then a green fluorescent polymer additive could EH-P was explored and it*s found that it could improve the air-illumination stability of these solar cells. The doped solar cells shown obvious advantaged performance compared than reference ones after 24-hours-illumination in air. Such a material shows great potential in real application and provides guidance in exploring new additive.

CPP 17.21 Mon 18:00 P3

Calculation of intra-molecular transition rates depending on structural parameters with DFTB — •Fabian Teichert, Robin Silligmann, Florian Günther, and Angela Thränhardt — Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany

Organic semiconductors become increasingly important for electronic applications. The large number of organic materials and their combinations make it useful to investigate properties like current-voltage characteristics using simulations in order to find suitable material combinations for applications. We investigate the transition rates of electrons between two organic molecules, expecially between thiophene, zinc porphyrin and PCBM. For this, we calculate HOMO and LUMO states and energies, reorganisation energies and Hamiltonian coupling matrices with DFTB using the software dftb+. Based on these results, the transition rates are computed using Marcus theory for charge transfer. We present result for two systems: (1) two thiophene molecules and (2) zinc porphyrin and PCBM. We show reorganisation energies, Hamiltonian coupling constants and transition rates dependent on the structural configuration. E.g. the thiophene molecules are shifted and rotated against each other. The final goal of our work is to obtain the statistical distribution of all the results due to the statistical fluctuation of the structure. This is suitable as input for subsequent Monte-Carlo hopping simulations, which can be used to describe the large-scale transport of charges within organic materials for e.g. solar cell applications.

CPP 17.22 Mon 18:00 P3

Charge transfer characteristics of an optically-driven conjugated molecular system — Vladyslav Savchenko and •Olga Guskova — IPF Dresden, Dresden, Germany

Recently [1], we have simulated E/Z isomers of two azobenzene-bithiophene (azo-bt) molecular switches in-between an anchoring surface and a gold STM tip. One of these switches has been previously synthesized [2], another one represents a structural isomer of [2], where azo and bt blocks have been swapped along the molecule. Here, we focus on the intermolecular charge transfer within chemisorbed monolayer because this aspect is still unexplored. First, DFT method is applied to define the reorganization energies for electron and hole transfer and the transfer integrals for stacked molecules using energy splitting in dimer approach. Further, the charge carrier mobility is evaluated. The results show, that the position of azo and bt favors either hopping of electrons or holes. For example, both isomers of the molecule with swapped blocks [1] are prone to the electron transfer, whereas for switch [2] the UV light stimulus toggles the main charge carrier from electron to hole. Interestingly, that molecule [2] possesses a non-zero mobility for the hopping distances h<0.5 nm, which requires densely packed layers. On contrary, relatively high electron transfer is predicted for molecule [1] even for sparsely anchored switches (h ca. 1 nm); the UV light turns off the hole hopping at distances h>0.5 nm as well. This work is supported by DFG, grant GU1510/5-1. [1] Savchenko V., Guskova O. Herald of TvSU. Series: Chem. 3(45) 2021, 7. [2] Karpe S., et al. Chem. Commun. 46, 2010, 3657.

CPP 17.23 Mon 18:00 P3

Critical Conditions in Transfer Matrix Methods — •Reinhard Sigel — Independent Scientist, Markdorf, Germany

The propagation of light in a layered refractive index profile is well described by transfer matrix methods (TMMs) [1]. Critical conditions (CC) occur when the wave vector perpendicular to the layering becomes zero. This case can be encountered in a total reflection geometry. Conventional TMMS become singular for CC. We discuss the divergence of layer amplitudes when one approaches CC. It is furthermore elucidated, how this divergence shows up in different experiments. New types of basis functions for a TMM based on virtually linear functions to circumvent the singularity have been introduced recently [2].

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CPP 17.24 Mon 18:00 P3

Surface doping of rubrene single crystals by molecular electron donors and acceptors — •Christos Gatsios[1], Andreas Opitz[1], Sebastian Hammer[3], Jens Pflaum[3], Yadong Zhang[4], Stephen Barlow[4], Seth R. Marder[5], and Norbert Koch[1,2] — [1]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany —

[3]Experimentelle Physik VI, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany — [4]Renewable and Sustainable Energy Institute (RASEI), University of Colorado, Boulder, CO 80309, USA — [5]Renewable and Sustainable Energy Institute (RASEI), Department of Chemical and Biological Engineering, Department of Chemistry, and Materials Science and Engineering Program, University of Colorado, Boulder, CO 80309, USA

Molecular doping can be used as a method to control the electronic energy levels and charge carrier densities of the organic semiconductor via charge transfer interactions with electron-donating or electron-accepting molecules. This work seeks to understand the mechanisms of interface engineering by focusing on the surface doping of rubrene single-crystals by molecular electron donors (CoCp2) and acceptors (Mo(tfd-CO2Me)3). Our angle-resolved photoemission results show that deposition of molecular dopants on rubrene shifts the valence band with respect to the Fermi level, thus changing the p- (n-) character of the surface, while the electronic band parameters remain essentially unaffected.

CPP 17.25 Mon 18:00 P3

Electronic structure of singlet fission donor-acceptor complexes — •Karin S. Thalmann[1], Pedro B. Coto[2], and Michael Thoss[1] — [1]Institute of Physics, University of Freiburg, Germany — [2]Spanish National Research Council (CSIC), Madrid, Spain

Singlet fission (SF) is a photophysical process in molecular materials describing the spin-allowed conversion of a singlet exciton to two triplet excitons [1]. Due to its ability to multiply charge carriers and its potential usage in solar cells to circumvent the Shockley-Queisser limit [2,3], SF has received significant attention recently. For future applications in energy conversion, the molecule exhibiting SF has to be combined with an electron acceptor to extract the energy of the two triplet excitons. As an example, we consider the complex of two covalently linked diazadiborine chromophore units as the SF exhibiting donor and tetracyanoquinodimethane as the acceptor molecule. Using multireference perturbation theory techniques, we analyze the electronic structure of the complex, in particular the electronically excited states, which include locally excited, charge transfer, and multiexcitonic states. Furthermore, we study the influence of the acceptor on the electronic structure of the donor molecule.

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CPP 17.26 Mon 18:00 P3

Recyclable-refabricated efficient solar cells with cellulose-based materials — •Shuxian Xiong[1,2], Marie Betker[1,3], Benedikt Sochor[1], Constantin Harder[1,2], Yusuf Bulut[1,2], L. Daniel Söderberg[3], Peter Müller-Buschbaum[2,4], and Stephan V. Roth[1,3] — [1]DESY, 22607 Hamburg, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [3]KTH Royal Institute of Technology, 10044 Stockholm, Sweden — [4]MLZ, TUM, Garching, Germany

Cellulose-based nanomaterials are used in a variety of potential applications, particularly in green electronics and optoelectronic devices, due to their sustainability, low cost and the ease of chemical functionalization. For recycling and prefabrications of cellulose-based solar cells, we propose the fabrication of green, fully sprayed solar cells based. The electrode material using conductive inks laminated with cellulose is easy to fabricate in large-area solutions. Preferably chlorine-free solvents are used in the active layer, and solvent engineering and post-treatment are used to control the morphology and aggregation to achieve high performance and environmental recyclability. The solar cells are planned to be recycled using the most environmentally friendly physical and chemical methods. The solar cell materials should be recycled to the maximum extent possible, and the recycled materials are then used to refabricate the solar cells and evaluate them in terms of morphology and efficiency.

CPP 17.27 Mon 18:00 P3

Towards needleless Electrospinning of a non-toxic, textile Dye-sensitized solar cell — •Marius Dotter — FH Bielefeld, University of Applied Sciences, Bielefeld, Deutschland

Photovoltaics can be used not only to feed energy into the power grid, but also to provide opportunities for applications on a smaller scale and for the autonomous supply of small electrical devices. In some cases, optimized efficiency can be dispensed with in favor of more cost-effective variants. Dye-sensitized solar cells (DSSC) offer a good option in this regard. They are also more effective indoors, because of a better conversion of stray light than semiconductor cells. Another idea is to make previously unused areas usable, with textiles such as tarpaulins, umbrellas and awnings being of particular interest. This niche, which has hardly been used so far, is to be filled by a textile DSSC, relying on needleless electrospinning for the textile haptics. This process, in which a polymer solution is formed into fine nanofibers using high voltage, which are then arranged in a disordered manner to form a nanofiber mat, enables simple and industrially scalable production of the DSSC components with a textile feel. In addition, simple production with non-toxic materials can also enable later reuse or simple recycling. In this context, this poster shows the general concept and progress of the work on the front electrode, which is based on a currently submitted paper.

CPP 17.28 Mon 18:00 P3

Exploring the kinetics of pseudo-bilayer architecture formation during sequential deposition via slot die coating — •Jinsheng Zhang[1] and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching — [2]MLZ, TUM, Garching

Recently, organic solar cells have received increasing attention due to obvious advantages such as flexibility and being lightweight. Among the different types of structures of the active layer, typically planar and bulk heterojunction geometries are used, which introduces intrinsic shortcomings. The newly developed pseudo-bilayer structure can perfectly combine their strengths and circumvent the drawbacks. Unfortunately, most of the pseudo-bilayer are still prepared by spin coating and rarely by printing methods such as slot die coating. Besides these studies mainly focus on selecting solvents, adding third components and studying the vertical morphology. The kinetics of forming the pseudo-bilayer architecture with slot-die coating are still unknown. Here we select the donor acceptor system PM6 and Y6 and the solvents CB and CF. First, PM6 is printed on the substrate and then Y6 is printed on top of PM6. During the deposition, in situ GIWAXS, in situ GISAXS, and in situ UV-vis absorption is carried out to study the formation of the pseudo-bilayer.

CPP 17.29 Mon 18:00 P3

Flash-lamp processing of charge extraction layers for polymer solar cells — •Aurelien Sokeng Djoumessi[1,2], Jose Prince Madalaimuthu[1,2], Shahidul Alam[1,2,3], Aman Anand[1,2], Anastasia Sichwardt[1,2], Peter Fischer[4], Roland Rösch[1,2], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldstrasse 10, 07743 Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany — [3]King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Physical Sciences and Engineering Division (PSE), Material Science and Engineering Program (MSE), Thuwal 23955-6900, Kingdom of Saudi Arabia — [4]Institute of Materials Engineering, Technical University of Ilmenau, Gustav-Kirchhoff-Str. 6, 98693 Ilmenau, Germany

Despite the benefits of thermal annealing (TA) in the fabrication of polymer solar cells, the high processing temperatures are not compatible with high throughput manufacturing techniques such as roll-to-roll, which commonly used flexible substrates. Therefore, techniques such as flash lamp annealing (FLA), which do not negatively affect the plastic substrate are needed. Herein, the FLA was successfully applied to PEDOT:PSS and SnO2 films used as interfacial layers in PM6:Y6-based solar cells, yielding device performances comparable to or even better than the devices treated with TA on a hotplate. Even at prototype size, the FLA is clearly more energy-efficient than the TA.

CPP 17.30 Mon 18:00 P3

Validating novel solar cells in space — •Lukas V. Spanier[1], Lennart K. Reb[1], Michael Böhmer[2], Christoph Dreissigacker[3], Zerui Li[1], Emanuel Anwander[1], Ahmed Krifa[2], and Peter Müller-Buschbaum[1,4] — [1]Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, Garching, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Central Technology Laboratory, Garching, Germany — [3]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Germany — [4]Technical University of Munich, Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany

The exploration of the outer solar system so far relied heavily on the use of scarce, highly radioactive plutonium stockpiles for power generation, as traditional solar cells have a too low power-to-mass ratio in low light environments to be suitable for those missions. Latest advances in organic and perovskite solar cells now open up the possibility of utilizing them on lightweight foils as photovoltaic solar sails for efficient power generation in low solar irradiation conditions.
We report the deployment of various organic and hybrid solar cell systems on a sounding rocket and their operation in outer space. We investigate the environmental influences during ascent, exposure to space, and reentry on the photovoltaic performance. We further study and compare the changes in morphology and optoelectronic behavior at various stages during the space mission, isolating different external impact factors.

CPP 17.31 Mon 18:00 P3

In situ study of superlattice self-assembly during slot-die coating of perovskite quantum dot films. — •David P. Kosbahn[1], Manuel A. Reus[1], Christopher R. Everett[1], Guangjiu Pan[1], Matthias Schwartzkopf[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching — [2]DESY, 22607 Hamburg — [3]Department of Fibre and Polymer Technology, KTH, Stockholm, Sweden — [4]MLZ, TUM, Garching

Research into quantum dots (QDs) of metal halide perovskites has become increasingly popular due to their stability and tunable optoelectronic properties. Their controllable surface chemistry and simple preparation make them a promising alternative to bulk perovskite solar cells. The power conversion efficiency of $Cs_xFA_{1-x}PbI_3$ QD solar cells has been steadily rising, up to a recent record efficiency of more than 16%. However, the alignment and self-assembly of the colloidal precursor into a superstructure during film fabrication via slot-die coating is not yet well-understood. In this work, we study the formation of perovskite QD films using in situ grazing-incidence X-ray scattering on different substrates and at different temperatures, to achieve a better understanding of the kinetic processes during solvent evaporation.

CPP 17.32 Mon 18:00 P3

Steady-State Microwave Conductivity (SSMC) on ionic liquid doped lead halide perovskites — •Patrick Dörflinger[1], Yong Ding[2], Mohammad Khaja Nazeeruddin[2], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Group for Molecular Engineering of Functional Materials, Institute of Chemical Sciences and Engineering, EPFL Valais, Sion 1950, Switzerland

Knowledge of the charge carrier lifetime and recombination behavior in perovskite solar cells is crucial, as non-radiative recombination processes still limit solar cell efficiencies. Here we present a technique to probe the charge carrier recombination. Of particular interest is the dominant charge carrier recombination pathway, which enables to quantify non-radiative recombination in the perovskite bulk. Furthermore, simultaneous photoluminescence measurements allow for estimating the doping density and determining the radiative efficiency at different charge carrier densities. As an example, the SSMC technique is applied to investigate the influence of ionic liquid additives, which are known to improve the stability of perovskite solar cells and the optoelectronic properties of perovskite absorbers.

CPP 17.33 Mon 18:00 P3

Giant Electrostriction in Lead Halide Perovskite $MAPbI_3$ Films as Measured with Double-Modulated Interferometry — •Philipp Ramming[1], Marvin Malchau[2], Emma Rauland[1], Anna Köhler[1], and Lothar Kador[2] — [1]Experimental Physics II, University of Bayreuth, Germany — [2]Institute of Physics and BIMF, University of Bayreuth, Germany

Hybrid lead halide perovskite semiconductor $MAPbI_3$ and similar materials have attracted much recent interest for photovoltaic devices. Upon application of moderate electrical fields, $MAPbI_3$ exhibits very large electrostriction effects. The thickness variation was measured with high precision using a double-modulation interferometer set-up. Phase modulation of the laser light and mechanical modulation of the interferometric path difference were employed. With field strengths on the order of 100 kV/cm, the relative thickness change of a polycrystalline film of 1 micron thickness can be as large as several per cent. The electrostriction varies with the square of the field strength; it is strongest at very low frequencies below one Hertz and decreases quickly at higher frequencies. The effect is compared to recently published data obtained on perovskite single crystals.

CPP 17.34 Mon 18:00 P3

First-principles study of the electronic and optical properties of perovskite solution precursors — •Freerk Schütt[1], Ana M. Valencia[1,2], and Caterina Cocchi[1,2] — [1]Carl von Ossietzky Universität, Institut für Physik, Oldenburg, Germany — [2]Humboldt-Universität zu Berlin und Iris Adlershof, Berlin, Germany

Metal halide perovskites have shown great promise for next-generation opto-electronic applications but the predominant employment of Pb poses a problem in terms of environmental sustainability of these compounds. Replacing Pb with Sn represents a viable solution, however, despite recent efforts in this direction [1], knowledge of Sn-based perovskites and precursors is to date still insufficient. In a first-principles work based on time-dependent density-functional theory coupled to the polarizable continuum model, we systematically investigate electronic and optical properties of SnI_2M_4 complexes, with M being common solvent molecules. We find that the structural, electronic, and optical properties are strongly affected by the choice of the solvent. By rationalising the behavior of 14 of such compounds even in comparison with lead-halide counterparts [2,3], we provide useful indications to complement experiments in the choice of the solvent molecules for SnI_2-based solution complexes and in their characterization towards the production of thin films [4].

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CPP 17.35 Mon 18:00 P3

In situ Grazing-Incidence Small-Angle X-ray Scattering Observation of TiOx Sputter Deposition on SnO2 Layer for Perovskite Solar Cells Application — •Xiongzhuo Jiang[1], Zhuijun Xu[1], Yusuf Bulut[1,2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]TUM School of Natural Science, Chair for Functional Materials, 85748 Garching, Germany — [2]Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany — [3]Department of Fibre and Polymer Technology, KTH, Stockholm, Sweden — [4]MLZ, TUM, 85748 Garching, Germany

It is crucial for the efficiency perovskite solar cells to promote the charge transport and suppress the non-radiation recombination in the hole blocking layer (HBL) and at the interface between the HBL and the active layer. Here, TiOx layers are deposited onto a SnO2 layer via sputter deposition at room temperature, forming a bilayer HBL. The structure evolution of TiOx during sputter deposition is investigated via in situ grazing-incidence small-angle X-ray scattering. After sputter deposition of TiOx with suitable thickness on the SnO2 layer, the bilayer HBL shows a suitable transmittance, smoother surface roughness, fewer surface defects and more suitable energy arrangement with active layer, and thus resulting in a lower trap-assisted recombination at the interface between the HBL and the active layer. With this SnO2/TiOx functional bilayer, the perovskite solar cells exhibit higher power conversion efficiencies than the unmodified SnO2 monolayer devices.

CPP 17.36 Mon 18:00 P3

Interfacial engineering via modifications of the electron blocking layer in PbS quantum dot solar cells — •Timo Piecuch[1], Huaying Zhong[1], and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]MLZ, TUM, Garching, Germany

Colloidal quantum dot solar cells (CQDSCs) have received tremendous attention as next generation solar cells. Best performances up to 15% power conversion efficiency (PCE) have been achieved using lead sulfide quantum dots in a heterojunction cell architecture. PbS is especially efficient in the infrared region, and thus particular interesting for future applications like space satellites. Research in the last years mainly has focused on improving the absorber layer and the hole blocking layer, but the potential by improving the electron blocking layer (EBL) has recently aroused increasing interest. In order to reduce interfacial charge carrier recombination and capture the large fraction of long wavelength photons at the EBL/active layer interface, the different interfacial energy-level offsets between EBL and absorber layer, tuned by the EBL-QDs size, are investigated using ultraviolet photoelectron spectroscopy (UPS) and absorption spectroscopy. Furthermore, the corresponding photovoltaic performances are characterized to demonstrate improved interfacial band alignment.

CPP 17.37 Mon 18:00 P3

PbS Quantum Dot Solar Cells for Space Applications — •Jasper Ebel[1], Huaying Zhong[1], and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]MLZ, TUM, Garching, Germany

A key performance parameter for photovoltaics (PVs) on space missions is the power-to-weight ratio since launch costs increase drastically with the mass-to-orbit. During the last decades, several promising, light-weight and flexible alternatives to current silicon- and GaAs-based technology have emerged, such as perovskite, organic or colloidal quantum dot (CQD) based solar cells. Lead sulfide (PbS) CQD solar cells are especially interesting due to their easily size-tunable bandgap range in the infrared regime, allowing for the exploitation of previously unused parts of the solar spectrum. This in conjunction with ligand, solvent and interface-customizable opto-electronic properties makes QD solar cells a promising candidate for tandem solar cells reaching high efficiencies. Here, by mimicking heat and illumination cycles experienced in orbit, we analyse the performance and structural integrity of PbS CQD solar cells under lab conditions to explore the viability of their use for space applications. Repeating this experiment for various solvents, we test a range of devices to investigate their effects on the stability.

CPP 17.38 Mon 18:00 P3

Hybrid Energy Harvester Based on the Combination of Triboelectric Nanogenerator and PbS Quantum Dot Solar Cell — •Tianxiao Xiao[1], Wei Chen[1], Wei Cao[1], and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]MLZ, TU München, 85748 Garching, Germany

Developing clean energy lies in the heart of sustainable development of human society. Triboelectric nanogenerator (TENG) originating from Maxwell's displacement current is a new type of energy harvester for harnessing ambient mechanical energy based on the coupling of triboelectrification and electrostatic induction effect. Compared with other counterparts, owing to the light-weight, low-cost, and easy fabrication, TENG has become one of the most promising candidates in replacement of conventional fossil fuels and attracted worldwide attention in the past years. However, to further increase the energy harvesting efficiency and broaden application fields, integrating the TENG with other kinds of energy harvesters in one device is a possible way to meet these needs. In the present work, a TENG based hybrid energy harvester is designed and fabricated on the flexible polyethylene terephthalate (PET) substrate. This hybrid device consists of a single-electrode mode TENG component and a PbS quantum dot (QD) based solar cell component, which can harness both mechanical and solar energy from ambient environment to directly generate electricity.

CPP 17.39 Mon 18:00 P3

Improved surface passivation of AgBiS2 quantum dots for photovoltaic applications — •Petar Lovric[1], Huaying Zhong[1], and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Heinz Maier-Leibnitz-Zentrum (MLZ), TUM, Garching, Germany

AgBiS2 colloidal quantum dots (QDs) are a non-toxic alternative for the commonly used PbS QDs for photovoltaic applications. Similar to its PbS QDs, they show great promise due to a tunable bandgap and solution processing, but what makes them stand out is the abundance of materials as well as a high absorption coefficient, which enables to greatly reduce the thickness of the active layer to around 35 nm. Additionally, studies have shown that they are more stable in water and can effectively harvest photons in the near-infrared part of the solar spectrum. One of major issue that impedes the development of AgBiS2 based photovoltaics is QD surface defects induced recombination losses. Here, we aim to improve the surface passivation of individual QDs and improve the charge transport in the QD films using surface ligand treatment with ZnI, mercaptocarboxylic acid (MPA) and TBAI as surface ligands. The optical and electrical properties of corresponding QDs films are characterized utilizing FTIR, XPS and UPS techniques, and further the corresponding device performances are investigated.

CPP 17.40 Mon 18:00 P3

Effect of ground state charge transfer and photoinduced charge separation on the energy level alignment at metal halide perovskite / organic charge transport layer interfaces — •Lennart Frohloff[1], Fengshuo Zu[1], Dongguen Shin[1], and Norbert Koch[1,2] — [1]Institut für Physik & IRIS Adlershof, HU Berlin — [2]Helmholtz-Zentrum Berlin

A proper energy level alignment at semiconductor interfaces is of paramount importance for realising high performance in perovskite solar cells. Therefore, we investigated the interface between a modern triple cation perovskite and a prototypical electron acceptor molecule in great detail. Strong band bending on both sides of the junction as well as negatively charged species of the organic molecule were evidenced by the means of photoemission spectroscopy, indicating a ground-state charge rearrangement across the interface. The band bending leads to significantly altered charge extraction offsets as compared to a hypothetical vacuum level alignment and flat band conditions. Additionally, we present direct evidence of a reversible reduction of the electron extraction offset under white light illumination as compared to the dark condition. The energy levels of the organic semiconductor were observed to rigidly shift to lower binding energy by up to 0.26 eV whilst the perovskite energy levels remain essentially unchanged. Consequently, we emphasise the necessity to determine the energy level alignment at interfaces involving perovskites not only in the electronic ground state but also under device operating conditions to allow for a reliable correlation to the performance of the device.

CPP 17.41 Mon 18:00 P3

Active layer aging for the fabricating durable perovskite solar cells with improved reproducibility — •Yuqin Zou[1] and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching — [2]MLZ, TUM, Garching

Solution processing of semiconductors is a highly promising approach for the fabrication of cost-effective electronic and optoelectronic devices. Although hybrid perovskites have potential in various device applications, challenges remain in the development of high-quality materials with simultaneously improved processing reproducibility and scalability. Here, we report a facile and practical aging treatment method to modulate crystal growth over the entire film to produces homogeneous films with high crystallinity, low defects and full-coverage. The resulting aged perovskite solar cells (PSCs) exhibits superior electronic properties: fast charge carrier transport, efficient charge extraction and low carrier recombination. The average power conversion efficiency (PCE) of MAPI-based PSCs greatly increase from 16.38% to 17.26% with high reproducibility. In addition, the aged PSCs maintain 80% of their initial PCE after 18 hours of operation under ambient and vacuum conditions, respectively, which illustrates their feasibility in scalable fabrication. Aging treatment effectively prevents the uneven performance and low reproducibility of PSCs arising from variations in the preparation environment (temperature, humidity). Thus, this method opens a new and effective avenue to improving the quality of perovskite films and photovoltaic devices in a scalable and reproducible manner.

CPP 17.42 Mon 18:00 P3

Investigating the Impact of Surfactants on Perovskite Film Formation Using In Situ Optical Spectroscopy — •Tobias Siegert, Simon Biberger, Konstantin Schötz, Anna Köhler, and Fabian Panzer — Soft Matter Optoelectronics (Experimental Physics II), University Bayreuth, Germany

Recent reports have shown that adding surfactants in the solution processing of halide perovskites, e.g. by blade-coating, can improve the morphology and optoelectronic properties of the resulting perovskite sample. In general, the crystallization processes of halide perovskites occuring during thin film formation largely determine the final film morphology. Thus, here we investigate the change in crystallization dynamics upon addition of surfactants to the precurser solution of halide perovskites. We monitor the film formation processes by multimodal optical in situ spectroscopy[1] to gain detailed insights about the film formation process of halide perovskites.[2-4] This finally allows us to elucidate the exact role and the impact of the presence of surfactants during solution processing on the crystallization behavior of the perovskite.

[1] Buchhorn, Wedler, Panzer. J. Phys. Chem. A 2018
[2] Chauhan, Zhong, Köhler, Panzer et al. J. Mater. Chem. A. 2020
[3] Schötz, Greve, Panzer et al. Adv. Optical Mater. 2021
[4] Biberger, Panzer et al. J. Mater. Chem. A. 2022

CPP 17.43 Mon 18:00 P3

Exploring the impact of nucleation seeds on the defect formation of printed hybrid perovskite films — •Altantulga Buyan-Arivjikh[1] and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching — [2]MLZ, TUM, Garching

In the research of next-generation solar technologies, perovskite-based devices are prominent candidates due to their lucrative power conversion efficiencies and ease of fabrication. Such devices typically contain a polycrystalline perovskite layer grown via various coating methods. Due to the short timeframe of the growth process, the formation of defects is inevitable, leading to increased non-radiative recombination- and decreased extraction of photogenerated charge-carriers. One route to counteract the extensive formation of defects would be the addition of external seeds in the precursor solutions, leading to more controlled nucleation and improved crystallinity of the thin film. In this study, different nucleation seeds in the precursor solutions were used for the fabrication of polycrystalline perovskite thin films via slot-die coating. The effect of the seeds on the formation of defects in the film was explored via optical spectroscopical methods such as UV-vis & PL spectroscopy.

CPP 17.44 Mon 18:00 P3

In-situ observation of growth mechanisms during printing of 2D perovskite films — •Kun Sun[1], Renjun Guo[1], Linus F. Huber[1], Manuel A. Reus[1], Jungui Zhou[1], Matthias Schwartzkopf[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]DESY, 22607 Hamburg, Germany — [3]Department of Fiber and Polymer Technology, KTH, SE-100 44 Stockholm, Sweden — [4]MLZ, TUM, 85748 Garching, Germany

Two-dimensional (2D) metal halide perovskites have emerged as a promising candidate for perovskite solar cells (PSCs) due to their remarkable stability compared with their 3D counterparts. However, solution-based spin-coating as fabrication method is not adequate in terms of upscaling. In this regard, the slot-die coating technique, having minimal expenditure and low costs, is a well suitable upscaling method to speed up the commercialization of PSCs. Nevertheless, a fundamental understanding of the film formation during printing is yet not well understood, which causes printed solar cells to stay behind in device efficiencies. Here, we investigate the nucleation and growth of 2D perovskite films during slot-die coating with in-situ grazing incidence wide angle X-ray scattering (GIWAXS) in combination with photoluminescence (PL) during printing. In addition, the crystallite orientation and phase distribution of 2D perovskite containing different dimensionality are well elucidated.

CPP 17.45 Mon 18:00 P3

Design, fabrication and application of PEO-based solid polymer electrolytes for all-solid-state lithium batteries — •Yingying Yan[1] and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Heinz Maier-Leibnitz-Zentrum (MLZ), TUM, Garching, Germany

All-solid-state lithium batteries (ASSLBs) have received extensive attention as one of the most promising power sources for flexible and wearable electronics, mainly because of their high flexibility, high energy density and reliable safety. However, the practical application of ASSLBs has been hindered by the poor interfacial stability and inferior ionic conductivity. Therefore, the exploration of advanced solid electrolytes with superior interfacial compatibility/ionic conductivity is an important research topic for all-solid-state batteries. Solid polymer electrolytes (SPEs) exhibit great potential in developing solid-state batteries, specifically for PEO and PEO-based derivatives, because of their superior interfacial compatibility, outstanding solubility against lithium salts, wide electrochemical windows and high ionic conductivity. At the same time, solid fillers, as an important component in SPEs, play a crucial role in determining the overall electrochemical properties. As a consequence, we start from PEO-based materials and prepare SPEs by adding plastic additives and solid fillers with good structure. The electrochemical performance and structural stability of SPEs are elucidated by a combination of electrochemical characterization and morphological structural characterization.

CPP 17.46 Mon 18:00 P3

Study of PEO Composite Electrolyte in All-solid-state Lithium Batteries — •Yuxin Liang[1], Zhuijun Xu[1], Kun Sun[1], Tianfu Guan[1], Fabian A.C. Apfelbeck[1], Pan Ding[2], Ian Sharp[2], Matthias Schwartzkopf[3], Stephan V. Roth[3,4], and Peter Müller-Buschbaum[1,5] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]TUM Walter Schottky Institute, Experimental Semiconductor Physics, Garching, Germany — [3]DESY, 22607 Hamburg, Germany — [4]KTH Royal Institute of Technology, Stockholm Sweden — [5]MLZ, TUM, 85748 Garching

Lithium batteries (LBs) with composite electrolyte present good ionic conductivity, flexibility and intimate contact with electrodes. However, lithium dendrites will grow and the Coulombic efficiency (CE) will decrease with Li plating and stripping. Moreover, the poly(ethylene oxide) (PEO)-based electrolyte undergoes serious oxidation on the cathode side at high voltage and cause the battery collapse. Strategies have been applied to alleviate the abovementioned challenges, nevertheless, fundamental research on the degradation mechanism of the PEO electrolyte is still lacking. It is of great value to get a deeper understanding and therefore optimize the electrolyte for high voltage LBs. Herein, we select PEO/Al2O3 as composite electrode to understand the degradation process. The Li/cathode cells are assembled to observe the battery performance and grazing incidence wide-angle X-ray scattering (GIWAXS) is used to detect morphology changes of the electrolyte before and after cycling.

CPP 17.47 Mon 18:00 P3

Influence of Al2O3 concentration in poly(propylene carbonate) based solid polymer electrolyte — •Thien An Pham[1,2], Ralph Gilles[1], and Peter Müller-Buschbaum[1,2] — [1]MLZ, TUM, Garching, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Solid polymer electrolytes (SPE) have emerged as promising electrolyte material group for all-solid-state batteries that allow the operation with Li metal anodes. Representing one of the main obstacles for Li metal anodes, Li dendrite growth can lead to short circuits which ultimately prevent the usage with liquid electrolytes. SPE offer higher mechanical stability compared to their liquid counterparts and thus, increase the general safety of Li metal batteries.

In this work, poly(propylene carbonate) based solid polymer electrolytes were synthesized with Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) as Li salt and varying Al2O3 concentrations via solution casting. The addition of Al2O3 has shown to increase the ionic conductivity of SPEs while simultaneously improve the mechanical stability. Furthermore, small angle X-ray scattering and FTIR were used to study the influence of Al2O3 on the structure of the SPE.

CPP 17.48 Mon 18:00 P3

Investigating Thermoelectric Properties of a Sodium-based, Solid Polymer-Electrolyte — •Julian-Steven Schilling, Maximilian Frank, and Jens Pflaum — Experimental Physics VI, University of Würzburg, 97074 Würzburg

Motivated by the large amount of available waste heat and the need to use energy more efficiently, the development of thermoelectric generators is becoming increasingly important. Their efficiency is characterized by the thermoelectric figure-of-merit z which includes the electrical conductivity σ, the thermal conductivity κ and the Seebeck coefficient S, respectively, and, at a given temperature T, is given by $zT = \frac{S^2\sigma}{\kappa}T$. In contrast to electronic thermoelectric materials, ionic systems promise larger Seebeck coefficients due to lower mobility of the participating charge carriers . Therefore, ionic electrolytes based on organic polymers are of interest due to their expected good thermoelectric performance. In this work, first results on the thermoelectric properties of a methacrylate-based solid polymer electrolyte utilizing sodium as conducting salt are presented. By means of impedance spectroscopy in a frequency range from 100 mHz to 500 kHz we analyzed the mechanisms governing the electrical conductivity in the technologically relevant temperature range from 273K to 353K. Complementary, thermovoltage measurements as function of temperature enable the determination of the Seebeck coefficient and, together with impedance spectroscopy data, reveal strategies how the electronic and ionic transport properties can be modified by the respective salt concentration as well as by the ratio of different carbon-based additives.

CPP 17.49 Mon 18:00 P3

In-situ force measurements on a gold working electrode in lithium-ion electrolytes — •Sabrina Kerz, Thomas Tilger, and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

Batteries have gained a great importance in recent years. They play a vital role in our every-day lives e.g. in mobile-devices and are an important pillar in the transition to renewable energies.

For these applications the solid electrolyte interface (SEI) at electrodes is of great interest. The Gouy-Chapman-Stern (CGS) model describes the interactions of the electrolyte with the charged electrode surface as an interplay between direct adsorption (Stern Layer) and a diffuse double layer. DLVO theory describes the diffuse double layer at the electrode's surface.

In-situ colloidal probe atomic force microscopy (CP-AFM) measures the force between a silica particle and the SEI. The obtained force curves are analyzed using DLVO theory. In a three-electrode setup different potentials are applied between a gold surface (working electrode) and a reference electrode. Thus, changes in the structure of the SEI with varying potentials and salt concentrations are examined.

CPP 17.50 Mon 18:00 P3

High-concentration Lithium-ion Electrolyte Overcomes the Challenges of High-temperature Lithium Batteries — •Tianle Zheng[1,2], Ya-jun Cheng[2], and Peter Müller-Buschbaum[1,3] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Ningbo Institute of Materials Technology & Engineering, CAS, Ningbo, 315201, P. R. China — [3]TUM, MLZ, 85748 Garching, Germany

Conventional Li-ion batteries are severely constrained in high-temperature applications due to the low thermal stability of the electrolyte/electrode interface and electrolyte decomposition in the cell. Herein, we demonstrate a new electrolyte that achieves an excellent stable long-term cycling at 100 °C, well beyond the typical 60 °C limits of normal conventional Li-ion batteries. High concentrated lithium oxalyldifluoroborate (LiODFB) is selected as the lithium salt with a carefully designed high thermal stability solvent group. As a result, this unique high-concentration electrolyte can promote to form a stable and inorganic solid electrolyte interface layer on the electrode at elevated temperature, leading to improved performance in MCMB/Li and lithium iron phosphate (LFP)/Li half-cells, and achieve reversible capacities of 160 and 350 mA h/g, respectively, with Coulombic efficiencies $> 99.3\%$. Subsequently, we further investigate the mechanism of high concentration LiODFB electrolytes by molecular dynamics simulations and XPS characterization techniques, exploring a new way for future high-temperature electrolytes.

CPP 17.51 Mon 18:00 P3

Morphology Control of Titanium Thin Films in a Low Temperature Process — •Guangjiu Pan[1], Shanshan Yin[1], Linus F. Huber[1], Caroline Ehgartner[2], Nicola Hüsing[2], Matthias Schwartzkopf[3], Stephan V. Roth[3,4], and Peter Müller-Buschbaum[1,5] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Universität Salzburg, 5020 Salzburg, Austria — [3]DESY, 22607 Hamburg, Germany — [4]KTH Royal Institute of Technology, SE 100 44 Stockholm, Sweden — [5]TUM, MLZ, 85748 Garching, Germany

A low-temperature routine to realize inorganic hole-blocking layers (HBLs) is important for the commercialization of perovskite solar cells. Fabricating HBLs at low temperature is energy-saving and compatible with flexible substrates. In this work, titania thin films are synthesized at low temperature (below 100 Celsius degree) with a polymer template sol-gel method based on the amphiphilic diblock copolymer polystyrene-b-polyethylene oxide (PS-b-PEO), in combination with selective incorporation of the titanium precursor ethylene glycol-modified titanate (EGMT). A joint process of UV treatment and water-vapor treatment is introduced to substitute the traditional high-temperature calcination. Morphology tailoring of titania thin films in the low-temperature process is achieved by managing phase separation of the polymer template. The surface morphologies of titania films are probed via scanning electron microscopy and GISAXS. The optical properties are examined with ultraviolet-visible spectroscopy and photoluminescence spectra.

CPP 17.52 Mon 18:00 P3

Bilayer formation in liquid-processed mono-functionalized BTBT films — Tim Hawly, •Andreas Späth, Manuel Johnson, Marcus Halik, Mingjian Wu, Erdmann Spiecker, and Rainer H. Fink — FAU Erlangen-Nürnberg, Erlangen, Germany

Two-dimensionally (2D) extended thin films of the p-type organic semiconductor C13-BTBT were fabricated by self-controlled growth at the water-toluene interface. Depicting a compound class originally developed for further functionalization and subsequent realization of self-assembled monolayers (SAMs) or their implementation into SAM-based organic field-effect transistors, the potent BTBT core unit commonly excels in high-quality structure formation as well as charge-transport characteristics. Utilizing various spectromicroscopic tools, we observe extraordinarily crystalline C13-BTBT films with a close to upright standing configuration of the BTBT backbone accounting for superior intermolecular orbital overlap. The well-defined morphology and internal structure of the film are underpinned by superior charge-transport parameters in corresponding OFETs. The inherently favorable membrane-like bilayer molecular arrangement is confirmed by the unambiguous representation of the unit cell as derived from STEM tomography. This study has been funded by the DFG within GRK 1896, the BMBF (contract 05K19WE2) and the Bavarian SolTECH initiative. [1] T. Hawly et al., ACS Adv. Energy Mat.(2022)/doi:10.1021/acsaelm.2c01095

CPP 17.53 Mon 18:00 P3

Characterization of pure DbSeQ thin films and their multilayers with different semiconductor materials — •Anton Pylypenko, Elena Chulanova, Alexander Gerlach, and Frank Schreiber — Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Organic semiconductor thin films are widely used in different areas of science and industry, especially for the manufacturing of organic optoelectronic devices. Bilayers of organic semiconductors are of high interest for research due to the possibility of increasing the advantages of blended materials [1]. Prospective candidates for these applications are derivatives of 2,1,3-benzothiadiazole, especially Dibenzoselenadiazoloquinoxoline (DbSeQ). The heavy atom has a strong impact on the spin-orbit coupling and thus the optical properties of the film. Understanding and investigating mechanisms of growth behavior is a key requirement for optimizing films.

We have investigated thin film growth and templating effects for various bilayers like DbSeQ:PIC or DbSeQ:DIP. The binary thin films are prepared by consistent evaporation of DbSeQ, DIP, and PIC on weakly interacting substrates under ultra-high vacuum conditions. Using ex-situ AFM, UV-VIS, and photoluminescence spectroscopies, X-ray reflectometry, and grazing-incidence wide-angle X-ray scattering, we have observed the morphology, structure, and crystallinity of bilayer films.

[1] A. Hinderhofer, F.Schreiber Chem Phys Chem (2012) 13 628

CPP 17.54 Mon 18:00 P3

Tunable morphologies in charged multiblock terpolymers in thin film geometry: effect of solvent vapor annealing — •Bahar Yazdanshenas[1], Florian A. Jung[1], Tim Bohnen[1], Sina Ariaee[2], Dorthe Posselt[2], Heinz Amenitsch[3], Constantinos Tsitsilianis[4], and Christine M. Papadakis[1] — [1]Technische Universität München, TUM School of Natural Sciences, Soft Matter Physics group, Garching, Germany — [2]Roskilde University, Department of Science and Environment, Roskilde, Denmark — [3]Graz University of Technology, Institute of Inorganic Chemistry, Graz, Austria — [4]University of Patras, Department of Chemical Engineering, Patras, Greece

Thin films of a pentablock terpolymer with an ABCBA architecture of two types of pH-responsive midblocks and short hydrophobic end blocks are investigated. As-prepared spin-coated films from different pH-values have previously shown highly tunable and non-monotonous behavior of the lateral structure sizes, based on the charge [1]. Here, we investigate further accessible morphologies by swelling the films in the vapors of solvents having different selectivity. Results from spectral reflectance, atomic force microscopy, and grazing-incidence small-angle X-ray scattering suggest that a solvent selective for the pH-responsive blocks leaves the nanostructures intact, while a nonselective solvent enables reorganization. Their vapor mixtures are also studied to potentially access further orientations and morphologies. In addition, an ABA triblock copolymer is investigated as a reference. [1] F. A. Jung, C. M. Papadakis et al., Adv. Funct. Mater. 2021, 31, 2102905.

CPP 17.55 Mon 18:00 P3

Computer simulations of liquids in extreme Confinement — •Luca Muigg[1], Gerhard Jung[2], Thomas Franosch[1], and Rolf Schilling[3] — [1]Institute for Theoretical physics, Universität Innsbruck, Innsbruck, Austria. — [2]Laboratoire Charles Coulomb (L2C), Université de Montpellier, CNRS, 34095 Montpellier, France. — [3]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany.

Computer simulations of a monodisperse hard-sphere liquid confined between two parallel hard walls of accessible width L are performed. By reducing the distance between the walls the two- dimensional limit $L \to 0$ is approached. An analysis of structural properties, such as the structure factor and the radial distribution function shows convergence to their two- dimensional counterparts, which is in agreement to the theoretical predictions. Furthermore an isobaric-like ensemble, with the slit width as an additional degree of freedom is introduced to study the behavior of the compressibility.

CPP 17.56 Mon 18:00 P3

Exploring the deposition conditions for formation of larger homogeneous colloidal arrays — •Joanne Neumann, Jan Rubeck, Andrei Chumakov, and Matthias Schwartzkopf — DESY, Photon Science, Notkestr. 85, D-22607 Hamburg

Installing regular arrays on mesoscopic length scales plays an important role in nanotechnology to create uniform templates for sputter deposition or plasma treatments. Different techniques of self-assembly via solvent evaporation out of dispersions have been used to obtain highly ordered colloidal structures. We used spin-coating, Langmuir-Blodgett (LB) technique and spray-deposition, representing the most attractive tools for the formation of larger homogeneous colloidal arrays on plain substrates. Due to their different deposition and boundary conditions, the assembly behaviour of polystyrene nanoparticles varies, resulting in two-dimensional layers with LB-technique and a large variety of pattern by spray deposition. We present our first results from atomic force microscopy and microbeam grazing incidence small-angle x-ray scattering (GISAXS).

CPP 17.57 Mon 18:00 P3

Incorporation of Nanomaterials to Form Electrically Conductive Multilayers with the Layer-by-Layer Technique — •Muhammad Khurram[1], Sven Neuber[2], Annekatrin Sill[3], and Christiane A. Helm[4] — [1]muhammad.khurram@uni-greifswald.de — [2]sven.neuber@uni-greifswald.de — [3]annekatrin.sill@uni-greifswald.de — [4]helm@uni-greifswald.de

Surface modification of an implant provides an adequate bio-interface and determines which promotes cell adhesion and proliferation. To promote healing, the coating should be electrically conductive. The Layer-by-Layer (LbL) method * sequential adsorption of oppositely charged macromolecules or nanoparticles - has become prominent in coating and functionalizing a surface. Polyelectrolytes show poor charge transfer capabilities; therefore, electrically conductive nanoparticles are essential. MXene nanoparticles are investigated. The MXene contains a high aspect ratio, functional groups, and good electrical conductivity. LbL films are built from polyanion MXene and polycation poly-diallyldimethylammonium (PDADMA). In addition, the conductive and conjugated polymers poly(3,4-ethylene dioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) is used because of their promising electrical properties. PDADMA is again the polycation. With the Atomic Force Microscope (AFM) film morphology and roughness are determined. Layer growth is monitored by UV-Vis Spectroscopy and ellipsometry. The electrical conductivity is determined with the two-point method.

CPP 17.58 Mon 18:00 P3

Band Gap Modification of 2D Covalent-Organic Frameworks (COFs) with Electron Rich and Electron Deficient Molecules — •Laura Fuchs, Konrad Merkel, and Frank Ortmann — School of Natural Sciences, Technische Universität München

A new type of porous materials are covalent-organic frameworks (COFs), which are suitable candidates as active substances for solar cells due to their highly tunable physical and electronic properties. Introducing electron rich (donor) and electron deficient (acceptor) regions to the molecular structure of 2D-COFs has an significant influence on the energetic levels of the highest occupied (HOMOs) and lowest unoccupied molecular orbitals (LUMOs). We provide insights to construction principles for band gap modifications by comparing the nature of the effect of widely-known electron acceptor and donor molecules[1] on the frontier electronic levels, as well as their impact on the charge density distribution using ab initio calculations within the density functional theory (DFT).

[1]Chua, M. H., Zhu, Q., Tang, T., Shah, K. W., & Xu, J. (2019). Diversity of electron acceptor groups in donor-acceptor type electrochromic conjugated polymers. Solar Energy Materials and Solar Cells, 197, 32-75.

CPP 17.59 Mon 18:00 P3

From a Completely Different Angle: Exploring Twistronicsin Layered Materials with Atomic Force Microscopy — •Alexander Klasen[1] and James Kerfoot[2] — [1]Park Systems Europe GmbH Schildkroetstrasse 15,68199 Mannheim, Germany — [2]Park Systems UK Limited, MediCity Nottingham Thane Road NG90 8BH, Nottingham, UK

Single atomic layer-based systems emerged as a promising class of materials with unique optical, mechanical, and electronic properties that could provide a pathway to novel applications.1,2 Their two-dimensional nature gives rise to a wide range of tunability since their functional properties do not only depend on the type of atoms and bonds within one plane but also on the strain, local defects, and interplay between adjacent layers.3,4 Here, we present Atomic Force Microscopy (AFM) based approaches as an ideal toolbox to map various functional properties of 2D materials and heterostructures on a nanometer scale. More specifically, by deterministically breaking and re-stacking single flakes of layered materials, we form homostructures of both hexagonal boron nitride (hBN) and molybdenum disulfide (MoS2) Investigating ferroelectric superlattices on a hexagonal boron nitride bilayer on a graphene single layer, we can induce domain switching when applying a constant DC potential and study them via Piezoelectric Force Microscopy.5,6 We will show how conductive AFM (C-AFM) and Lateral Force Microscopy (LFM) allow imaging strain variations as distorted domains in both the current channel and the lateral force channel.

CPP 17.60 Mon 18:00 P3

Lieb lattice embedded in square polymer — •Yingying Zhang, Miroslav Položij, and Thomas Heine — Faculty of Chemistry and Food Chemistry, TU Dresden, Dresden, Germany

Dirac cone and flat band are exotic band features, which attracted much attention in these years, in which the movement of charge carriers is massless fermions, leading to ultra-high carrier mobility and various quantum Hall effects. Structure in lieb lattice owns these two intriguing bands simultaneously, characterized by one dispersive Dirac band inserted with a flat band, which may give rise to many exotic quantum phenomena such as ferromagnetism, topological states, or superconductivity.

The theoretical TB model predicted that the idea lieb band requires rigorous lattice symmetry and zero next-nearest neighbor (NNN) hopping, making the lieb band rarely found in real materials except widely studied via TB model or photonic and cold-atom. There are only two synthesized structures with lieb band were reported.

Therefore, I studied a systematic square phthalocyanine COF with a defined length of linkers, showing that the lieb band is embedded in square polymer. The Pc-xBz COFs show how the band evolution between square and lieb is based on a series of structures with extending linkers. The band structure and charge density distribution are analyzed to further study the electronic properties. We also show that, by charge doping and atom replacement, the fermi level can be tailored to the lieb band position, making the structure intriguing and potential.

CPP 18: Organic Electronics and Photovoltaics I (joint session CPP/HL)

Time: Tuesday 9:30–13:00 Location: GÖR 226

CPP 18.1 Tue 9:30 GÖR 226

Use of a multiple hydride donor to achieve an n-doped polymer with high solvent resistance — Farzaneh Saeedifard[1,2], Dominique Lungwitz[3], Zi-Di Yu[4], Sebastian Schneider[5], Ahmed E. Mansour[3,6], •Andreas Opitz[3], Stephen Barlow[1,2], Michael F. Toney[1], Jian Pei[4], Norbert Koch[3,6], and Seth R. Marder[1,2] — [1]University of Colorado Boulder, US — [2]Georgia Institute of Technology, Atlanta, US — [3]Humboldt-Universität zu Berlin, Germany — [4]Peking University, China — [5]Stanford University, US — [6]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

Insolubilization of doped semiconducting polymer layers can help to fabricate efficient multilayer solution-processed electronic and optoelectronic devices. Here, we present a promising technique to simultaneously n-dope and largely insolubilize conjugated polymer films using tetrakis[4-(1,3-dimethyl-2,3-dihydro-1*H*-benzo[*d*]imidazol-2-yl)phenoxymethyl]methane (tetrakis-O-DMBI-H), which consists of four 2,3-dihydro-1*H*-benzoimidazole (DMBI-H) n-dopant moieties covalently linked to one another. [1] Doping a thiophene-fused benzodifurandione-based oligo(*p*-phenylenevinylene)-*co*-thiophene polymer (TBDOPV-T) with tetrakis-O-DMBI-H results in a highly n-doped film with bulk conductivity of 15 S/cm. Optical absorption spectra reveal a film retention of $\sim$93% after immersion in *o*-dichlorobenzene for 5 min. This is caused by multiple electrostatic interactions the multiple electrostatic interactions between each dopant tetra-cation and up to four nearby anionic doped polymer segments.

[1] F. Saeedifard et al., *ACS Appl. Mater. Interfaces* **14** (2022) 33598.

CPP 18.2 Tue 9:45 GÖR 226

Numerical Simulation of Crystallization Kinetics in Binary Mixtures for Organic Photovoltaic Applications — •Maxime Siber, Olivier Ronsin, and Jens Harting — Helmholtz-Institute Erlangen-Nürnberg for Renewable Energies (HI-ERN), Germany

With the aim to understand the formation process of organic photoactive layers, and identify process-structure relationships in order to optimize their fabrication, a computational framework relying on the phase-field modelling approach has recently been developed. It is now sought to quantitatively compare numerical simulations of drying organic photovoltaic (OPV) films with corresponding experimental realizations.

Since the fabrication process involves the interplay of multiple physical phenomena, which separate characterization already is a challenging task from the simulative, as well as from the experimental side, this first study focusses on crystallization behaviour in isothermal, non-evaporating, binary OPV blends. In particular, this talk addresses crystalline structures that arise from different crystallization processes such as solution-triggered crystallization, diffusion-limited crystallization, or spinodal decomposition-assisted crystallization. Furthermore, crystallization kinetics quantified for several blend ratios and material parameters are also analyzed and compared. Finally, perspectives regarding validation against in-situ experiments and derivation of design rules for OPV film fabrication are also provided.

CPP 18.3 Tue 10:00 GÖR 226

Optical properties of perfluorotetracene (PFT) crystal polymorphs — •Ana Maria Valencia[1,2] and Caterina Cocchi[1,2] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg — [2]Physics Dept., Humboldt-Universität zu Berlin und IRIS Adlershof

The family of perfluorinated acenes is gaining popularity among organic materials for optoelectronics. Since the electronic and optical properties of molecular solids are crucially dependent on their packing motifs, it is crucial to consider crystalline phases in the simulations to understand the structure-property relationships of these materials, especially regarding electronic correlations and excitations. Here, we investigate from first principles by means of density functional theory and many-body perturbation theory the electronic structure and the optical excitations of two crystal polymorphs of perfluorotetracene, considering for comparison tetracene and the corresponding isolated molecules. This way, we can assess the effects of fluorination as well as of the crystal periodicity. We find that the absorption spectra are only mildly influenced by the packing motif. However, our analysis gives insight into the exciton binding energies as well as the spatial distribution of the excitons. We inspect not only the first excitations but also the higher-energy ones, thus providing an all-around understanding of the optical excitations in these materials.

CPP 18.4 Tue 10:15 GÖR 226

Controlling long-range order in dip coated piezo- and ferroelectric molecular materials — •Andrey Butkevich and Martijn Kemerink — Institute for Molecular Systems Engineering and Advanced Materials, Im Neuenheimer Feld 225, 69120 Heidelberg, Germany

Organic piezo- and ferroelectrics are of great interest due to their tunable properties. However, the extensive procedures that are often required to achieve saturation polarization limit their possible applications. A so far unexplored possible solution is to pre-align the molecules during the deposition from solution. Here, we analyzed the effect of dip coating parameters on the alignment of multiple supramolecular piezo- and ferroelectrics. Dip coated films were characterized for different material concentrations and dip coating velocities. The investigation revealed that morphologies with strong alignment along the dip coating direction are formed for both material types. For ferroelectrics, the changes in the ferroelectric switching behavior of the resulting thin films were investigated. The ferroelectric switching was investigated using the double wave method, revealing that dip coating perpendicular to the electrodes leads to an almost perfect in-plane alignment of the supramolecular polymers, which was confirmed by X-ray diffraction. The observed switching behavior was comparable to films that were aligned via conventional field-annealing. Hence, dip coating enhanced the ferroelectric switching in the investigated molecules, which we anticipate can be directly transferable to other molecular ferroelectrics.

CPP 18.5 Tue 10:30 GÖR 226

In search of novel organic ferroelectrics — •Heiko Mager — IMSEAM, Heidelberg University

The switchable polarization and concomitant pyroelectric and piezoelectric properties of ferroelectric materials enable a variety of applications, ranging from memory devices over thermal and mechanical sensors to energy harvesters. Although current applications are dominated by inorganic materials, organic ferroelectrics offer a flexible, cheap and possibly non-toxic and biodegradable alternative.

Here, we present experimental research on the ferroelectric-like behavior of the novel liquid crystalline molecule C6H6F5O-C3-Amide and its molecular derivatives. To screen for a possible para- to ferroelectric phase transitions, dielectric spectroscopy was employed. While the for ferroelectric materials characteristic Curie-Weiß behavior was not directly observed, features in the dielectric suggest a possible phase transition coinciding with a peak in differential scanning calorimetry traces.

Polarization hysteresis loops were obtained via double wave measurements and characteristic capacitance- voltage "butterfly" loops measured. Comparisons between the different molecular derivatives allow insights into the molecular groups relevant for the switching process.

CPP 18.6 Tue 10:45 GÖR 226

Implementation and simulation of drift-diffusion models for organic mixed conductor devices — •Andres David Peña Unigarro[1,2] and Florian Steffen Gunther[2,3] — [1]Institute of physics, TU Chemnitz, Chemnitz, Germany — [2]IFSC, University of São Paulo, Brazil — [3]UNESP, Rio Claro, Brazil

Organic electrochemical transistors (OECTs) have emerged as potential transducers in applications that require the conversion of ion fluxes to electronic current. For the understanding of the fundamental mechanism in OECTs and OECT-based applications, as well as for their rational optimization, however, it is essential to have theoretical models that agree with experimentally measured device responds. Most of the existing OECT models consider that the ion flux from the electrolyte into the organic, semiconducting layer takes place only due to an electrical field. These models are efficient to describe the steady state operations of OECTs, but are rather limited when compared to transient behaviors. Recently, more refined models which take a diffusion term into account, have been developed. The simplifications needed to use an analytical solution of the governing equation, however, reduces its generality, limiting the results to specific cases. In our work, we use numerical methods to solve the drift-diffusion equation in one dimension to overcome these limitations of the analytical solution. This allows us to go beyond the standard boundary conditions and to analyze the impact of other alterations.

CPP 18.7 Tue 11:00 GÖR 226

Noise in Organics Semiconductors and Devices — •Priya Viji, Dorothea Scheunemann, Constantin Tormann, and Martijn Kemerink — Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University, Germany

Noise, typically considered an unwanted signal in measurements, can also contain information about the charge kinetics in organic semiconductors. Since the corresponding devices often show high resistances and capacitances, the measurement of -albeit very small- current fluctuations via voltage noise is most suitable. To quantify this noise and to eliminate noise from other devices in the measurement line, a cross-correlation technique is implemented and applied to P3HT doped with varying concentrations of F4TCNQ. The results compare quantitatively with kinetic Monte Carlo simulations in which noise calculations were implemented. To understand the effect of the electric field on the charge carriers, disentangling noise in directions parallel and perpendicular to the electric field is essential. The direction perpendicular to the electric field does show a gradual increase at high electric fields, which matches the concept of an Effective Temperature, as described by Marianer and Shklovskii, in which the effects of electric field and lattice temperature are combined. In the direction of the electric field, an additional contribution due to shot noise is observed. However, its magnitude deviates from the theoretical prediction of shot noise, which can be quantified as a non-unity Fano-factor.

15 min. break

CPP 18.8 Tue 11:30 GÖR 226

Uniaxially Aligned Merocyanine Films by Graphene Nanoribbon Templated Growth — •Philipp Weitkamp, Lukas Böhner, Nora Gildemeister, Dirk Hertel, and Klaus Meerholz — Physikalische Chemie, Universität zu Köln, Deutschland

We herein report the unique and novel approach of achieving a polycrystalline thin film consisting of uniaxially aligned domains by using 7-armchair graphene nanoribbon (7-aGNR) monolayers as van-der-Waals template. For this purpose, a merocyanine dye was evaporated on 7-aGNRs, transferred on quartz glass substrates. The alignment of the formed molecular aggregate along the GNR alignment direction was proven by polarisation dependent absorbance spectroscopy. The J- and H-transition, formed by the dye aggregate, were correlated with distinct axes of the crystal structure. By combining this correlation with polarisation dependent absorbance measurements and X-ray diffraction experiments we elucidated the three-dimensional structure of the formed aggregate thin film. The growth mode of these films was investigated as a function of the applied layer thickness. Atomic force microscopy-based morphology analysis and X-ray diffraction experiments were used to reveal the anisotropic on-surface crystallisation along the 7-aGNR long axes direction. Furthermore, we found that the delocalisation length of the aggregate increases with increasing in-plane order. Finally, we demonstrated that the in-plane alignment leads to an anisotropic charge carrier transport by implementing the templated merocyanine thin film as active layer in a top-gated organic field effect transistor.

CPP 18.9 Tue 11:45 GÖR 226

Investigation on organic light-emitting diodes, fabricated by a self-developed and highly automated physical vapor deposition system — •Fabian Binder, Mona Löther, Pascal Schady, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Organic light emitting diodes (OLEDs) are most commonly produced in ultra-high vacuum by physical vapor deposition (PVD) of several organic and metallic layers on a carrier substrate. We developed an automated PVD system, mainly consisting of two vacuum chambers for organic and metal deposition, respectively. Stepper motors and sensor solutions ensure a smooth and precise positioning of the carrier substrate above the evaporation crucibles. The substrate is then rotated with a defined speed to achieve an even deposition of the material. In order to vapor-deposit material, a certain material-specific temperature range is required which is realized by a software-based temperature controller which manages the evaporation rate according to the user's specifications. A user interface facilitates planning of the desired OLED layer stack and provides information about the production progress. The capabilities of our new PVD system were tested by producing OLEDs based on multiple-resonance TADF emitters of the DABNA series. We performed electro-optical LJV-characterization and determined the devices'quantum efficiencies. The results of this investigation will enable us to optimize the production process with regard to evaporation rates and layer thicknesses.

CPP 18.10 Tue 12:00 GÖR 226

improvement of electrical transport in organic semiconductor thin films by charge transfer doping — •Hongwon Kim[1], Andreas Opitz[2], Florian Fenzl[1], and Wolfgang Brütting[1] — [1]Experimentalphysik IV, Institut für Physik, Universität Augsburg — [2]Institut für Physik, Supramolekulare Systeme, HU zu Berlin

Charge carrier transport in organic semiconductor is based on the hopping mechanism. We have used in-situ charge transfer doping during film-growth to improve the electrical conductivity by simultaneously increasing the carrier density and reducing their thermal activation energy. By doping planar organic semiconductors, such as DBTTF, a-6T, and DIP, with strong acceptors (F6-TCNNQ & HATCN), hybridization of pi-orbitals occurs while generating new interphases (charge transfer complex, CTC). On the other hand, DBP, a non-planar molecule, forms an amorphous thin film without any CTC generation. To measure the characteristics of CTC, we used near-infrared transmission spectroscopy, which can detect the absorption peaks of CTCs and the energy gap. In addition, the activation energy is obtained from temperature-dependent conductivity measurements. We observe a correlation between the magnitude of the electrical conductivity and its activation energy, which can be ascribed to the binding energy of CTCs. Depending on the specific system, conductivity maxima are observed between 10 and 30% molar doping ratios.

CPP 18.11 Tue 12:15 GÖR 226

Electrical transport dynamics of conducting polymers in nanoconfinement — Sukanya Das and •K.S. Narayan — Chemistry and Physics of Materials Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru- 560064, India

Inherently disordered conducting polymers consist of different characteristic lengths, defect distribution over the polymer chains and their microstructural modifications can alter the transport properties significantly. The electrical transport of conducting polymers such as poly(3,4-ethylene dioxythiophene): poly(styrenesulfonate) PEDOT:PSS has shown conductivity enhancement when confined in an array of nanochannels in the form of alumina nanopillars. The transverse conductivity along the nanopillar axis, which is an otherwise suppressed quantity, increases nonlinearly by approximately three orders in magnitude as the diameter of the scaffold-channel is decreased to 20 nm, when measured at single nanochannel level as well as at bulk-macroscopic level. This suggests the major role of dimensions and geometry in eliciting efficient electrical transport. Similarly, more than 3 orders of conductivity increase have been shown by in-situ polymerized poly(3,4-ethylenedioxythiophene):tosylate within the nanochannels which has similar electronic backbone PEDOT but a different dopant environment. The microscopic insight into PEDOT:Tos has shown higher degree of crystallinity and ordering as compared to PEDOT:PSS nanochannels. We utilize this property of PEDOT:PSS to fabricate hybrid organic-inorganic perovskite photodiode with efficient hole extraction and faster response times in the nanoconfined devices.

CPP 18.12 Tue 12:30 GÖR 226

In-situ spectro-electrochemistry of N-type conjugated organic systems for opto-electronic and electro-optic applications — •Meenal Kataria and Sabine Ludwigs — IPOC-Functional Polymers, Institute of Polymer Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany

This talk will highlight our ongoing research on in-situ spectroelectrochemistry. We are developing functional organic conjugated materials and devices for opto-electronic and electro-optic applications. Here, one of our aims is to utilize an in-situ spectroelectrochemical approach to calculate the energy levels of blends of donor polymers (e.g. PM6) and non-fullerene acceptors (e.g. Y6) utilized for high performance organic solar cells. For relevant device information it is important to have precise values of energy levels of the same blend systems as used in devices. Thus, our absorption assisted electrochemistry technique proved be advantageous approach (1). In another research work discussing the effect of isomerism on conductivity of n-type polymers (e.g. P(NDI2OD-T2)), this above approach has been used to identify the redox states during electrochemical doping which helped to identify the charge transfer transport mechanism (2). In the last example, this technique has been utilized to calculate the frontier energy levels of push-pull D-π-A systems and to study the effect of acceptor strength on their energy levels (3).

Ref. (1) J. Mater. Chem. C 2022, 10, 11565. (2) Chem. Mater. 2019, 31, 3542. (3) Phys.Chem.Chem.Phys. 2020, 22, 2283.

CPP 18.13 Tue 12:45 GÖR 226

Delocalization Enhances Conductivity at High Doping Concentrations — •Dennis Derewjanko[1], Dorothea Scheunemann[1], Emmy Järsvall[2], Anna I. Hofmann[2], Christian Müller[2], and Martijn Kemerink[1] — [1]IMSEAM, Heidelberg University, Im Neuenheimer Feld 225, 69120 Heidelberg, Germany — [2]Department of Chemistry and Chemical Engineering, Chalmers University of Technology, 41296 Gothenburg, Sweden

Many p-type organic semiconductors are experimentally found to follow a universal power-law trend between conductivity and charge carrier concentration at practically relevant high doping levels. This behavior cannot consistently be explained by conventional charge transport models. Here, we develop a physically transparent model based on the combination of a tight binding model and a variable range hopping model to show that the observed power-law trend can be explained by consideration of an energy dependent localization length. The underlying cause is an energetic lifting of the charge carriers to partly delocalized states due to the rising Fermi energy level at high charge carrier concentration. At low charge carrier concentrations, the well-known Mott-Martens model is recovered.

CPP 19: Crystallization, Nucleation and Self-Assembly

Time: Tuesday 9:30–13:00 Location: MER 02

Invited Talk CPP 19.1 Tue 9:30 MER 02

Multiscale Model of Flow-Induced Crystallization in Polymers — David Nicholson, Marat Andreev, Chenmay Gangal, and •Gregory Rutledge — Massachusetts Institute of Technology, Cambridge, MA USA

The structure and properties of a semicrystalline polymer depends sensitively on both its chemico-physical nature and the way it is processed. Flow-induced crystallization (FIC) is one such coupled phenomenon. Models of FIC in polymers must account for the effect of flow on crystallization kinetics, but also the effect of evolving crystallinity on the rheology of the flowing polymer melt. For the first part, atomistic nonequilibrium molecular dynamics (NEMD) simulations are used to characterize the nucleation of a new crystal phase from the polymer melt under homogeneous flow conditions. The kinetics of nucleation are characterized using a mean first-passage time analysis, and a model based on the orientational ordering of Kuhn segments is proposed. For the second part, a variation of the discrete slip-link model (DSM) is used for the rheology of entangled polymer melts that accounts for partial crystallinity through the introduction of crosslinked *bridge* and/or *dangling* segments between developing crystallites, combined with a suspension model to reflect the stiffening associated with a growing crystal phase. This dual-network/suspension model describes well the evolution of both viscoelasticity and crystallinity for a number of linear low-density polyethylenes, and affords a deeper understanding of the essential physics that underlie the coupling between fluid mechanics and phase change.

CPP 19.2 Tue 10:00 MER 02

Polyethylene crystallization induced by a solution-prefolded nucleus — •Timur Shakirov and Wolfgang Paul — University of Halle, Halle, Germany

We present results of molecular dynamics simulations of an undercooled polyethylene melt. We simulate a system of 2000 chains of 150 monomers each with the PYS force-field [1]. To initiate crystallization we insert in the melt a small two-chain nucleus (which we pre-fold in the vacuum) and cool down the system to 280 K. The crystalline lamella forms around the inserted nucleus during the cooling process and grows further at constant temperature. We characterize the growing crystallite by its average diameter (typical linear size in the cross-section perpendicular to the crystal director) and the height of the lamella (the averaged size along the crystal director). Both, diameter and height of lamella, grow during the entire simulation (~ 900 ns at the final temperature). A saturation of the growth is observed only as the crystallite reaches the surrounding spontaneously formed crystallites. Our analysis of the chain kinetics in the inner volume of the crystallite shows remaining chain mobility along the chain director. The distribution of short-time displacements of the inner-crystalline monomers has signatures of discrete jumps of a single bond length along the director of the crystal.

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

CPP 19.3 Tue 10:15 MER 02

How to grow semicrystalline lamellae in MD simulations — William Fall[1,2], Jörg Baschnagel[1], Olivier Lhost[3], and •Hendrik Meyer[1] — [1]Institut Charles Sadron, CNRS UPR22 and Université de Strasbourg, France — [2]LPS Université Paris-Saclay, Orsay, France — [3]TotalEnergies One Tech Belgium, Zone Industrielle C, 7181 Feluy, Belgium

To investigate the influence of short chain branches in the crystallization of high molecular weight polyethylene (PE) we adapted a united monomer model for molecular dynamics simulations. We showed recently that a small fraction of branches allows to control the lamellar thickness in the semicrystalline structures [Macromol **55** (2022) 8434]. This work is extended to bidisperse mixtures of highly entangled C_{4000} and C_{400} with different branch distributions mimicking industrial PE morphologies. A self-seeding protocol is presented which allows to simulate the growth of well aligned lamella, and analyse morphological features. We thank TotalEnergies for funding and GENCI/IDRIS (Orsay) and CAIUS/HPC centre (Strasbourg).

CPP 19.4 Tue 10:30 MER 02

Crystallization precursors in polymer melt analyzed by machine learning — •Atmika Bhardwaj[1,2], Marco Werner[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e. V., Hohe Str. 6, D-01069 Dresden, Germany — [2]Institute for Theoretical Physics, Technische Universität Dresden, Zellescher Weg 17, D-01069 Dresden, Germany

Crystallization in polymers is a long-standing problem in both experimental and theoretical polymer science. The transition dynamics occurring in an under-cooled polymer melt is a local environmental phenomenon rather than a property of individual particles (or monomers) and depends on subtle conformation patterns such as entanglements between the chains. We develop machine learning (ML) methods to study this non-equilibrium thermodynamic process. Upon recognizing the relevant parameter set to explore different phases during polymer crystallization, we investigate the spatial and temporal patterns of the precursor states that determine the nucleation sites. The objective is to recognize the precursors that stimulate crystal growth before the occurrence of such development.

CPP 19.5 Tue 10:45 MER 02

How entanglements determine the morphology of semicrystalline polymers — Zefan Wang, Mareen Schaller, Albrecht Petzold, Kay Saalwächter, and •Thomas Thurn-Albrecht — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle

Crystallization of polymers from entangled melts generally leads to the formation of semicrystalline materials with a nanoscopic lamellar morphology. Controlling this structure is key to the rational design of thermoplastic materials, but there is no consensus yet on the factors that control the thickness of the amorphous layers and therefore together with the crystal thickness the crystallinity. We here elucidate the effect of entanglements on the morphology in a series of model blends of high-molecular-weight polymers with unentangled oligomers leading to a reduced entanglement density in the melt as characterized by rheological measurements. Small-angle X-ray scattering experiments after isothermal crystallization reveal a reduced thickness of the amorphous layers, while the crystal thickness remains largely unaffected. A simple yet quantitative model without adjustable parameter is suggested, according to which the measured thickness of the amorphous layers adjusts itself in such a way that the entanglement concentration reaches a specific maximum value.

CPP 19.6 Tue 11:00 MER 02

Modelling Study of Reinforcement and Crack Formation in Strain-Crystallizing Elastomer Networks — •Lena Tarrach[1], Reinhard Hentschke[1], and Jan Weilert[2] — [1]Bergische Universität Wuppertal, Wuppertal, Germany — [2]Covestro Deutschland AG, Leverkusen, Germany

A coarse-grained model has been developed to simulate reinforcement and crack formation in strain-crystallizing elastomer networks. This work is based on the model for strain-induced crystallization (SIC) proposed by Plagge and Hentschke [1], which here is extended for the investigation of rupture.

Generally, strain-crystallizing elastomer networks possess a higher tensile strength than non-crystallizing networks. Therefore, the force on the links, i.e. the polymer chains in the model network, is analyzed to define a critical force for their rupture. It is examined how structural parameters and parameters for the free energy of semi-crystalline links affect the tensile strength of strain-crystallizing networks compared to non-crystallizing networks. The variation of these parameters does not improve the tensile strength in both the 2D- and the 3D-case.

Thus, a critical crystallinity, which makes certain links unbreakable, is introduced to model the alignment of the polymer backbones along the stretching direction. The tensile strength of 2D- and 3D-networks is enhanced.

[1] Plagge, J. & Hentschke, R. Microphase Separation in Strain-Crystallizing Rubber. *Macromolecules* **54**, 5629-5635. https://doi.org/10.1021/acs.macromol.1c00757 (2021).

15 min. break

CPP 19.7 Tue 11:30 MER 02

New experimental setup to analyze structure formation in thermoplastic polymer melts — •Anna Katharina Sambale[1], Eric Euchler[1], Regine Boldt[1], Kai Uhlig[1], Laura Neumann[1], Konrad Schneider[1], Matthias Schwartzkopf[2], Stephan Roth[2,3], and Markus Stommel[1,4] — [1]Leibniz-Institut fuer Polymerforschung, Dresden, Germany — [2]Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — [3]KTH Royal Institute of Technology, Stockholm, Sweden — [4]Technical University Dresden, Dresden, Germany

The microstructure of semi-crystalline thermoplastics is significantly influenced by the processing procedure and its parameters. Inhomogeneous shear and extensional flow fields occurring during processing can cause constraints to the chain conformations, which in turn lead to altered crystallization behavior. Although the influence of crystallization kinetics on the properties of the most commonly used polymers is considered to be sufficiently known, (local) conditions and parameters in commercially used melt processing technologies are not fully understood. We recently started to develop a new experimental setup to study structure formation in polymers induced by melt processing. The first results on the crystallization processes in quiescent polymer melts under isothermal conditions investigated by X-ray scattering measurements will be presented. In particular, time- and temperature-dependent crystallization of polylactic acid (PLA) and isotactic polypropylene (iPP) with different crystallization rates were examined and proved the concept of the experimental setup.

CPP 19.8 Tue 11:45 MER 02

The missing billions in hard sphere nucleation — Sahana Kale, Nidhi Joshi, and •Hans Joachim Schöpe — Universität Tübingen, Institut für angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Crystal nucleation in colloidal hard spheres is a longstanding research topic in colloidal science. Light scattering experiments as well as simulations have been carried out to determine key parameters characterizing the nucleation process and to get a microscopic picture of the fluid to crystal transformation. In these studies, results both differ and agree with each other. It is still unclear whether the large disagreement in the nucleation rate densities between the experiments and simulations are of physical nature or result from different data analyses. Using laser-scanning confocal microscopy and polarization microscopy we study crystal nucleation in colloidal hard spheres. The used systems have been characterized with extreme care to allow for meaningful comparison with other experiments and simulations. We present high quality data of the nucleation rate density and key parameters describing crystal nucleation. Analyzing the nucleation process we conclude that classical nucleation theory fails.

CPP 19.9 Tue 12:00 MER 02

Non-metallic quasicrystals minimize sphere packing energy — •Martin Dulle[1], Vladislava Fokina[1], Thomas Gruhn[2], and Stephan Förster[1] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Universität Bayreuth, Bayreuth, Germany

Quasicrystals are a peculiar state of order, which is fundamentally different from classical ordered crystalline states. Discovered in 1982 for metal alloys, they have in recent years also been reported for an increasing number of non-metallic materials.

Using MD-simulations we calculate the phase diagram of soft repulsive core/shell particles and find stability regions for seven different octagonal, decagonal, dodecagonal and icosahedral quasicrystals. We compare the structure and stability region of the dodecaganol phase with experiments on different polymer and nanoparticle systems and find quantitative agreement. We identify a new high density dodecagonal phase in a large number of reported non-metallic quasicrystalline systems including polymers, mesoporous silica, surfactants, BaTiO3, TaTe and MnCrNiSi. All remaining reported non-metallic quasicrystals can be related to the other simulated quasicrystal types.

We geometrically derive all respective tilings and show how in-plane quasicrystalline order is combined with axial periodic order via the realization of certain gyro-elongated bipyramids. This geometrical arrangement minimizes sphere packing energy for certain length scale ratios and particle densities, irrespective of the absolute length scale, the type of interactions and chemical constituents.

CPP 19.10 Tue 12:15 MER 02

Controlling internal structure of colloidal supraparticles - crystalline to amorphous — •Yashraj Wani[1], Melis Yetkin[2], Michael Kappl[2], Hans-Jürgen Butt[2], and Arash Nikoubashman[1] — [1]Institute of Physics, JGU Mainz, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany

Colloidal supraparticles made from smaller nanoparticles (NPs) are versatile materials whose properties can be tailored through the chemistry and ordering of their constituent NPs. Such supraparticles can be scalably fabricated using solvent-drying processes that assemble NPs inside liquid droplets. In charge stabilized dispersions, the interactions can be controlled by the salt concentration, which we systematically probed in experiments and simulations. In experiments at low salt concentrations, the dried supraparticles exhibited high crystalline order, whereas amorphous structures were found at high salinity. To understand this evaporation-induced structure formation, we first determined the interaction potentials between NPs via colloidal probe atomic force microscopy and dynamic light scattering experiments. Using these pair potentials, we carried out particle-based simulations to study the aggregation behavior in detail: At low salt concentrations, the effective NP-NP interactions remained purely repulsive until the end of drying, resulting in highly crystalline supraparticles. At higher salt concentrations, however, the electrostatic repulsion became screened, leading to the formation of small NP aggregates at early stages of drying, which then eventually merged into an amorphous supraparticles.

CPP 19.11 Tue 12:30 MER 02

Unravelling the synthesis of halide perovskite nanoplatelets by SAXS — •Kilian Frank[1], Carola Lampe[2], Alexander S. Urban[2], and Bert Nickel[1] — [1]Soft Condensed Matter Group and CeNS, Faculty of Physics, LMU Munich — [2]Nanospectroscopy Group and CeNS, Nano-Institute, Faculty of Physics, LMU Munich

Halide perovskite nanoplatelets (NPLs) are a promising material for optoelectronic applications, such as LEDs and single photon emitters. While highly scalable and reliable ligand-assisted synthesis routes exist, a detailed structural understanding of the underlying pathways is lacking. We elucidate the processes of nucleation, growth, and superstructure assembly of CsPbBr3 NPLs using in situ small-angle X-ray scattering (SAXS), total scattering (TS) and photoluminescence (PL) spectroscopy during the synthesis. Thereby we enable even better control of the platelet thickness on the monolayer level, and therefore of the emission wavelength, due to quantum confinement. For this purpose we built and used a specialized reaction cell for in situ synthesis at the beamlines P07 and P62 (PETRAIII, DESY, Hamburg). By SAXS analysis we follow the assembly of the constituents into a regular superstructure. In addition, we investigated the effect of post-synthetic treatment of the NPLs using the same setup to further enhance their optoelectronic properties. With our results we contribute to the development of assembly-based synthesis routes for size-tunable nanomaterials. Such materials are of particular interest to the perovskite community as building blocks for hierarchical structures.

CPP 19.12 Tue 12:45 MER 02

From protein adsorption to crystallization: a simultaneous real-time QCM-D and microscopy study — •Hadra Banks, Furio Surfaro, Simon Storz, Anna Maischberger, Cara Buchholz, Kai-Florian Pastryk, Alexander Gerlach, and Frank Schreiber — University of Tübingen, Germany

Protein crystallization is widely investigated by employing a homogeneous nucleation approach; however, it is predicted that heterogeneous nucleation is energetically more favorable [1]. Nevertheless, only few experimental studies on the nucleation of protein crystals at surfaces are available, since this is a complex phenomenon and requires surface-sensitive techniques. Here, quartz crystal microbalance with dissipation monitoring (QCM-D), a real-time surface-sensitive technique, was employed simultaneously with optical microscopy to investigate protein adsorption and crystallization at a negatively charged surface. Human serum albumin (HSA) and β-lactoglobulin (BLG), in the presence of a trivalent salt, were used as model systems for the study of heterogeneous nucleation [2]. We found that their surface behavior during crystallization exhibit complex phenomena such as wetting transition, enhanced adsorption, and layer rearrangements. The results highlight the importance of the interaction between proteins and surfaces and how this can influence protein phase behavior.

[1] J. R. Espinosa et al., Soft Matter 15 (47), 9625-9631, 2019

[2] O. Matsarskaia et al., ChemPhysChem 21 (16), 1742-1767, 2020

CPP 20: Polymer and Molecular Dynamics, Friction and Rheology

Time: Tuesday 9:30–12:30 Location: ZEU 255

Invited Talk CPP 20.1 Tue 9:30 ZEU 255

Granular Matter Rheology – fluid-/solid-like behavior and state-transitions — •Stefan Luding — University of Twente, NL

The dynamic and static behavior of particulate and granular matter (like sand, powder, suspended particles, often with a wide distribution of particle sizes) is of considerable interest in a wide range of industries and research disciplines. Special is that they can behave both solid-like and fluid-like, which is a challenge for both academia and industry. The related mechanisms/processes in particle systems are active at multiple scales (from nano-meters to meters), and explaining their multiple states, and transitions, will lead to a better understanding of natural disasters like avalanches or industrial problems like silo-failure.

To understand the fundamental micro-mechanics and -physics, one can use particle simulation methods. However, large-scale applications (due to their enormous particle numbers) have to be addressed by coarse-grained models or by continuum theory. For this, to derive constitutive rheology relations, so-called micro-macro transition methods are necessary, which translate particle positions, velocities and forces into density-, stress-, and strain-fields, which must be compatible with the balance equations for mass, momentum, and energy of continuum theory. Additional non-classical fields describe the microstructure (fabric, force-chains) or the statistical fluctuations,before an universal granular rheology can be defined, involving state-transitions between the states, the so-called jamming/un-jamming transitions.

CPP 20.2 Tue 10:00 ZEU 255

Phase-Sensitive, Active Microrheology via Probe-Free Application of Thermoviscous Flows — •Iliya Stoev, Elena Erben, Venkat Krishnaswamy, Antonio Minopoli, Susan Wagner, Benjamin Seelbinder, Nicola Maghelli, and Moritz Kreysing — Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstraße 108, 01307, Dresden, Germany

We recently found how thermoviscous expansion phenomena give rise to a new, contactless particle trap that is characterised by a linear force-extension relationship and can therefore be employed in non-invasively measuring femtoNewton forces with thermally limited sensitivity. Our new force-measurement method is based on optically generated flows, thereby lifting prerequisites related to the probe material and resulting in only moderate heating at the position of the micromanipulated object. This methodology offers an appealing alternative to the use of optical tweezers in highly delicate samples and living systems. Next, we asked the question if our thermoviscous flows can be used to obtain more quantitative data and possibly demonstrate the equivalence between flow-driven and force-driven rheology in their ability to extract phase angles as a measure of relative mechanics. With our new flow-based and phase-sensitive microrheology, we provide access to the mechanics of highly viscous media, tenuous gels and even cellular cytoplasm. Further refinements of the method aim at multiplexing and removing the need for using fluorescent tags.

CPP 20.3 Tue 10:15 ZEU 255

Nanoscopic Friction on Monolayer MoS_2 in Presence of Water Investigated with Molecular Dynamics — •Miljan Dašić and Igor Stanković — Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

We have implemented and applied a molecular dynamics (MD) simulation setup in order to study the nanoscopic friction on monolayer MoS_2 plate in the presence of different quantities of water. Our setup mimics a standard AFM experiment, including an amorphous SiO_2 probe, a monolayer crystalline MoS_2 plate, and water molecules in-between. Presence of water molecules matches experimental conditions of air humidity. We studied two different quantities of water: (1) *full water layer* - SiO_2 probe is fully immersed in water and surrounded by water molecules, and (2) *capillary water* - water forms a capillary around the SiO_2 probe, with lateral vacuum gaps. We conducted two modes of simulations: vertical approach of SiO_2 probe towards MoS_2 plate and lateral sliding of SiO_2 probe. There are always *trapped* water molecules in the gap between the probe and the plate; their number drops with the increase of temperature. We have obtained well-pronounced *stick-slip* friction loops; we found that an increase of the applied normal load leads to the more pronounced stick-slip behaviour, as seen in AFM experiments. The amount of water present in the studied nanoscopic tribosystem has a pronounced impact on the stick-slip frictional behaviour.

CPP 20.4 Tue 10:30 ZEU 255

Polymers of Intrinsic Microporosity - Molecular Mobility and Physical Aging Revisited by Dielectric Spectroscopy and X-Ray Scattering — •Farnaz Emamverdi, Glen Jacob Smales, Martin Böhning, and Andreas Schönhals — Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205 Berlin, Germany

The applications of polymers of intrinsic microporosity (PIMs) membranes are restrained by their strong tendency to physical aging. Aging phenomenon involves a significant loss of their good performance in gas separation technology. The initial microporous structure approach a denser state via local rearrangements, leading to a reduction of the permeability. In this work, the dielectric behavior of PIM-1 films and their behavior upon hating (aging) were revisited by isothermal frequency scans during different heating/cooling cycles over a broad temperature range between 133 K and 523 K. In addition, the obtained results were compared with data of samples that were annealed at ambient temperatures over different time scales. Multiple dielectric processes were observed: several relaxation processes due to local fluctuations and a Maxwell-Wagner-Sillars polarization effect related to microporosity. The temperature dependence of the rates of all processes follows the Arrhenius law where the estimated activation energy depends on the nature of the process. SAXS/WAXS patterns were measured as a function of temperature during heating/cooling in a temperature range corresponding to that covered by dielectric spectroscopy. The influence of the aging on the processes is discussed in detail.

CPP 20.5 Tue 10:45 ZEU 255

Viscoplastic Modeling of Surface Relief Grating Growth on Isotropic and Pre-oriented Azopolymer Films — Tverdokhleb Nina[1], Loebner Sarah[2], Santer Svetlana[2], and •Marina Saphiannikova[1] — [1]Institute Theory of Polymers, Leibniz Institute of Polymer Research Dresden, 01069 Dresden, Germany — [2]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany

We report on solving two intriguing issues concerning the inscription of surface relief gratings within azopolymer thin films under irradiation with SS, PP and RL interference patterns. For this, we utilize the orientation approach and viscoplastic modeling in combination with experimental results, where the change in surface topography is acquired in-situ during irradiation with modulated light. First, the initial orientation state of polymer backbones is proved to be responsible for the contradictory experimental reports about the efficiency of the SS interference pattern. Different orientation states can influence not only the phase of SS grating but also its height, which is confirmed experimentally using special pre-treatments. Second, faster growth of gratings inscribed by the RL interference pattern is shown to be promoted by a weak photo-softening effect. Overall, the modeled results are in good agreement with the order of relative growth efficiency: RL-PP-SS.

CPP 20.6 Tue 11:00 ZEU 255

Equilibration of free-standing films of highly entangled polymer melts — •Hsiao-Ping Hsu and Kurt Kremer — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128, Mainz, Germany

Equilibrating confined and free-standing films of highly entangled polymer melts is a challenge for computer simulations. We approach this problem by first studying polymer melts based on a soft-sphere coarse-grained model confined between two walls. The distance of the walls is compatible with the simulation box of bulk melts in equilibrium, while periodic boundary conditions in the directions parallel to the walls are kept. Then we successively insert more fine grained polymer representations until the underlying microscopic details of the bead-spring model are reached. Tuning the wall potential, the monomer density of confined polymer melts in equilibrium is kept at bulk melt density even near the walls. Switching to another recently developed variant of the bead-spring model we can study melts at zero pressure [1] and study free-standing polymer films [2]. Furthermore, this also allows us to study free-standing films under strain and analyze the influence of entanglements on the local film morphology.

[1] H.-P. Hsu, K. Kremer, J. Chem. Phys. 150, 091101 (2019); 150, 159902 (2019).

[2] H.-P. Hsu, K. Kremer, J. Chem. Phys. 153, 144902 (2020); 156, 019901 (2022).

15 min. break

CPP 20.7 Tue 11:30 ZEU 255

A nanofluidic system based on cylindrical polymer brushes: molecular dynamics simulation and scaling theory — •Cheng-Wu Li — Leibniz-Institut für Polymerforschung Dresden, Germany

Using molecular dynamics simulations and scaling theory, we present a systematic study of the function of cylindrical nanopores which are decorated with polymer brushes. Our focus is on the regimes in which these systems are able to function as controllable (switchable) gates for bulky nanoparticles. In a slightly poorer solvent, closed cylindrical brushes facilitate the self-organised formation of droplets from a continuous flow of incoming nanoparticles We analyze droplet formation and propagation by means of simple scaling arguments which are tested in the simulations. Polymer brushes in marginally poor solvents serve as a pressure feedback system, exhibit a collapse transition under the moderate pressure of the incident flow, without the need for additional external stimuli, and finally close spontaneously after droplet passage. Our results qualitatively demonstrate the control of polymer brushes over continuous fluids and droplet formation, and its effectiveness as a means of fluid control can be used to design nanofluidic rectification devices that operate reliably under moderate pressure.

CPP 20.8 Tue 11:45 ZEU 255

Polymer chain dynamics under shear studied by rheological NMR — •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

The NMR spin-lattice relaxation time T2 is particularly sensitive to slow chain-segment motion in polymers, at least two components in the signal decay are observed, a faster relaxing component from chain segments of motion restricted by crosslinks or entanglements and a slower component associated with parts moving more freely. Ordering of the polymer chains under shear would result in restrictions for the segment motion and thus a shortening of T2, a loss of entanglements due to the shear results in a prolongation of T2. Rheological NMR combined external shear with NMR experiments. In a polymer melt of poly(dimethylsiloxane) under shear longer relaxation times are observed. Together with a reduction of the fraction of shorter T2 this indicates the loss of entanglements is the dominating process for high molecular weight. In a new experimental setup both the amplitude and the frequency of the deformation are varied. It demonstrates that a minimum strain rate above 1000/s is required to observe the loss of entanglements. Combining pulsed-field-gradient (PFG) NMR with NMR imaging permits to measure flow pattern. After the turning point in oscillatory shear counterflow is observed when a fraction of the liquid at the static wall still is in initial flow direction while liquid in contact with the moving bob started in the new direction. At this time the velocity gradient drastically exceeds the velocity gradient at the point of maximum velocity representing a high shear rate.

CPP 20.9 Tue 12:00 ZEU 255

On the Relaxation Behavior of Linear Chains under Oscillatory Forces — •Ron Dockhorn[1] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institut für Theoretische Physik, D-01069 Dresden, Germany

We are studying the relaxation spectra and the force-extension behavior of linear chains under externally driven oscillatory periodic forces f in means of theory and simulations. An oscillatory force $f = f_0 + f_a \cdot \sin(\omega t)$ is applied on the chain ends and the response of the end-to-end-distance R as well as the relaxation time τ_R on the oscillatory frequency ω is investigated. An analytical expression for the end-to-end-distance $R(f)$ is derived by using the Rouse model and compared to simulations. The dissipated energy is calculated by the hysteresis loop $A = \left|\oint df R(f)\right|$, which shows a characteristic maximum at $\omega\tau_R \simeq 1$ for ideal chains independent of the applied force. Contrary, excluded volume chains show a force dependence on the relaxation time $\tau_R \sim f^{-0.3}$ as well as a shift on the hysteresis in the Pincus regime. Extensive computer simulations are performed to investigate the scaling properties utilizing the Bond-Fluctuation-Model. Furthermore, the relaxation behavior of different polymer architectures (ring polymer, 3_1-trefoil knot, two concatenate rings) are compared to the linear chain behavior. The theory and simulations suggests implications for dynamic experiments of biopolymer subject to external forces.

CPP 20.10 Tue 12:15 ZEU 255

Orientation Polarization Spectroscopy — •Friedrich Kremer, Wycliffe Kipnusu, and Markus Anton — Leipzig University, Peter Debye Institute for Soft Matter Physics,Linnéstr.5,04103Leipzig,Germany

The theory of orientation polarization and dielectric relaxation was developed by P. Debye more than 100 years ago. It is based on approximating a molecule by a sphere having one or more dipole moments. By that the detailed intra- and inter-molecular interactions are explicitly not taken into consideration. In this contribution the principal limitations of the Debye approximation are discussed and novel experiments based on Quantum Cascade IR-Lasers are presented [1] which enable to determine the orientation polarization of selected molecular moieties for the example of the glass forming liquid glycerol. [1] Kremer, F. et al. Int. J. Mol. Sci. 23, 8254 (2022)

CPP 21: Active Matter III (joint session BP/CPP/DY)

Time: Tuesday 9:30–12:30 Location: TOE 317

CPP 21.1 Tue 9:30 TOE 317

Gliding motility and reorientation of flagellated microbes on curved surfaces — •Alexandros Fragkopoulos[1], Nicolas Fares[1,2], and Oliver Bäumchen[1] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]University of Bordeaux, CNRS, LOMA, UMR 5798, 33400 Talence, France

The model organism *Chlamydomonas reinhardtii*, a unicellular biflagellated microalga, can adhere and colonize almost any surface under particular light conditions. Once the cells attach to a surface, an intraflagellar transport machinery translocates the cell body along the flagella, which are oriented in a 180° configuration. This motion is known as gliding motility. Even though the cells firmly adhere to surfaces, they are able to reorient through different physical mechanisms [1]. With the use of the orientation autocorrelation function, we find that cells exhibit large reorientation events shortly after their initial attachment to a surface, while at longer time scales they are primarily constrained to 1D motion. On cylindrical surfaces, the large reoriations cause the cells to predominantly align in the direction of the minimum principle curvature. We quantify the curvature-induced alignment using the nematic order parameter and reveal that the minimum surface curvature required for cell alignment is comparable to the static flagella curvature.

[1] S. Till, et al., *Phys. Rev. Res.*, (Accepted)

CPP 21.2 Tue 9:45 TOE 317

Efficiency of navigation strategies for active particles — •Lorenzo Piro[1], Ramin Golestanian[1,2], and Benoit Mahault[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, United Kingdom

Optimal navigation in complex environments is a problem with multiple applications ranging from designing efficient search strategies to engineering microscopic cargo delivery. When motion happens in presence of strong external forces, route optimization is particularly important as active particles may encounter trapping regions that would substantially slow down their progress.

Here, considering a self-propelled agent moving at a constant speed, we study the efficiency of Zermelo's classical solution. Investigating both cases of motion on the plane and on curved surfaces, we focus on the regime where the external force exceeds self-propulsion in finite regions. There, we show that, despite the fact that most trajectories following the trivial policy of going straight get arrested, the Zermelo policy allows for a comprehensive exploration of the environment.

However, our results also indicate an increased sensitivity of the Zermelo strategy to initial conditions, which limits its robustness and long-time efficiency, particularly in presence of fluctuations. These results suggest an interesting trade-off between exploration efficiency and stability for the design of control strategies to be implemented in real systems.

CPP 21.3 Tue 10:00 TOE 317

Run with the Brownian Hare, Hunt with the Deterministic Hounds — •Davide Bernardi[1] and Benjamin Lindner[2,3] — [1]Italian Institute of Technology, Ferrara, Italy — [2]Bernstein Center for Computational Neuroscience, Berlin, Germany — [3]Institut für Physik, Humboldt-Universität zu Berlin

Pursuit and evasion are vital to most animal species and play an important role in many human activities. Traditionally, chase-and-escape models have been studied in the framework of game theory, or in detailed models that can be studied only through numerical simulations and that lack generalization power.

Here, we present analytic results for the mean time and energy used by a pack of deterministic hounds to capture a prey that undergoes Brownian diffusion. Depending on the number of chasers, we find that the mean capture time as a function of the prey's diffusion coefficient can be monotonically increasing, decreasing, or attain a minimum at a finite value. Furthermore, an optimal speed and number of chasing hounds exist, that depend on the baseline power consumption and drag coefficient of each chaser.

The present model can be seen as an analytically tractable basis for the theoretician's perspective on the growing field of smart microswimmers and autonomous robots.

CPP 21.4 Tue 10:15 TOE 317

Function of Morphodynamics in Foraging *Physarum polycephalum* — •Lisa Schick[1], Mirna Kramar[2], and Karen Alim[1] — [1]School of Natural Sciences, Technical University of Munich, Germany — [2]Institute Curie, Paris, France

How network-forming fungi structure and reorganize their network morphology and thereby the carbon flows in the soil is key to understanding climate - yet hidden from us due to the long time scales of network dynamics and the soil itself. Here, the network-forming slime mold *Physarum polycephalum* serves as a model of network dynamics of a foraging network-forming life. We follow and quantify the network migration velocity and morphology of foraging *P. polycephalum.* We identify three distinct morphological states characterized by network compactness and density of moving fronts. Estimating the energetic cost of distinct states, we find that morphological variability allows the organism to balance the energetic costs of foraging and search strategy. Our observations allow us to project how resource availability might shift the balance and thereby affect network extension in foraging network-forming organisms.

CPP 21.5 Tue 10:30 TOE 317

Unraveling the migratory behavior of a large single-celled organism — •Lucas Tröger, Florian Goirand, and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

Many cells face search problems, such as finding food, conspecifics, or shelter, and different search strategies can provide different chances for success. In contrast to most single-celled organisms the slime mold *Physarum polycephalum* forms a giant network-shaped cell while foraging for food. Which advantage does the giant cell at the verge to multicellularity provide? We experimentally investigate and quantify the long-time migratory behavior of small networks of *P. polycephalum* in the absence and in the presence of food, and develop a simple mechanistic model that successfully describes its migration. We find that *P. polycephalum* performs a run-and-tumble-like motion modified by self-avoidance to achieve superdiffusive migration. Furthermore, it tunes its short-time dynamics in order to adapt to environments with different amounts of available nutrients, while its long-time dynamics remain unchanged. This work shows how *P. polycephalum* controls the inherent stochasticity of its movement by simple rules, which may represent an evolutionary advantage.

15 min. break

CPP 21.6 Tue 11:00 TOE 317

Controlling active turbulence by activity patterns — •arghavan partovifard, josua grawitter, and holger stark — Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Active fluids exhibit spontaneous and chaotic flow patterns which are known as active turbulence [1]. One of the current challenges in active matter is controlling and harnessing these flow patterns for powering processes at small scales [2]. As a simple realization of an active fluid, we consider a semi-dilute solution of active rods and study it within a numerical simulation of the governing equations that are formulated in terms of velocity and the orientational order tensor parameter fields.

We find that for a solution of pusher active rods there is a critical magnitude of activity above which the initially isotropic solution develops locally varying nematic order and turbulent-like fluid flow. Aiming to control the turbulent flow state, we pattern the activity with a square lattice of circular inactivity spots. We find that for a specific range of lattice parameters the flow field develops lanes of unidirectional flow with alternating directions while between them a row of corotating vortexes emerges; We call this state the laning state and it is multistable since different realizations of the random initial state of rods lead to different configurations of the laning state with various widths of the lanes. In this state, the director field develops nematic domains oriented toward the Leslie angle with respect to the flow.

[1] Wensink *et al.*, Proc. Natl. Acad. Sci. **109**, 14308-14313 (2012)

[2] Bowick *et al.*, Phys. Rev. X **12**, 010501 (2022)

CPP 21.7 Tue 11:15 TOE 317

Active matter: From spontaneous to controlled phenomena.

— •Daniel Pearce — University of Geneva

Active matter is the study of materials able to move themselves. During this talk I will discuss how we can take advantage of the interplay between topological defects, geometry and topology to exercise control over active materials. By studying active nematic fluids on a curved surface, we can influence the position and orientation of topological defects according to their charge. This means specific nematic textures can be generated. By studying active contractile actomyosin gels, it is possible to show that only active topological defects with charge +1 can generate curvature, and the sign is related to the phase of the defect. This frees the process from the constraints of the Poincare-Hopf theorem and allows complex surfaces to be generated. This is demonstrated by recreating the shape of a freshwater hydra from the positions of the topological defects

CPP 21.8 Tue 11:30 TOE 317

Nucleation of chemically active droplets — •Noah Ziethen and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Liquid-liquid phase separation emerged as a crucial organizing principle inside biological cells giving rise to a plethora of intracellular compartments. Unique to the cellular context, these condensates can consist of only a few hundred molecules and are affected by non-equilibrium processes. In particular, active chemical conversion between condensate material and proteins in the surrounding cytoplasm can control multiple aspects of the condensates. Yet, it is unclear how these reactions affect the spontaneous nucleation and dissolution associated with low particle numbers. Here, we investigate the influence of chemical reactions on the bistable region of active droplets using a stochastic field theory. We find an effective increase in the energy barrier and thus decelerated transitions between the homogeneous and the droplet state. Using classical nucleation theory, we approximate the full dynamics by diffusion in a free energy potential described by an analytical expression only depending on droplet radius and reaction rate. This analogy also allows us to determine the equivalence of the binodal line, so we can propose an extension of the equilibrium phase diagram to capture driven chemical reactions. Cells might use these effects to control the nucleation of intracellular droplets.

CPP 21.9 Tue 11:45 TOE 317

Hydrodynamic description and transport coefficients in a model of active cellular aggregates — •Subhadip Chakraborti[1,2] and Vasily Zaburdaev[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

Complex multicellular aggregates consisting of a large number of interacting cells are ubiquitous in biology, ranging from bacterial biofilms to organoids, cell spheroids, and tumors. We consider colonies of *N. gonorrhoeae* bacteria as a prototypical example of cells that use retractile cell appendages to actively interact with a substrate and with each other. We construct a microscopic model on a 1D lattice taking into account the non-equilibrium bacterial motility driven by two crucial forces – cell-substrate and cell-cell interactions. We observe a phase transition from a homogeneous state to a clusterized state upon tuning the density and activity parameters. Using macroscopic fluctuation theory (MFT), we analytically derive hydrodynamics for the model system and calculate two density-dependent transport coefficients – the bulk-diffusion coefficient and the conductivity. The behavior of these transport coefficients successfully explains the non-equilibrium phase transition. We support our analytical findings with the results obtained numerically. Our theory provides a general framework for studying the non-equilibrium collective behavior of other dense cellular aggregates also, in the context of dynamics and their transport properties.

CPP 21.10 Tue 12:00 TOE 317

Flocking of unfriendly species: The two-species Vicsek model — •Swarnajit Chatterjee[1], Matthieu Mangeat[1], Chul-Ung Woo[2], Heiko Rieger[1], and Jae Dong Noh[2] — [1]Saarland University, Saarbrücken, Germany — [2]University of Seoul, Seoul, Korea

We consider the two-species Vicsek model (TSVM) consisting of two kinds of self-propelled particles, A and B, that tend to align with particles from the same species and to anti-align with the other. The model shows a flocking transition that is reminiscent of the original Vicsek model [1]: it has a liquid-gas phase transition and displays micro-phase separation in the coexistence region where multiple dense liquid bands propagate in a gaseous background. The novel feature of the TSVM is the existence of two kinds of bands, one composed of mainly A-particles and one mainly of B- particles and the appearance of two dynamical states in the coexistence region: the PF (parallel flocking) state in which all bands of the two species propagate in the same direction, and the APF (anti-parallel flocking) state in which the bands of species A and species B move in opposite directions. When PF and APF states exist in the low-density part of the coexistence region they perform stochastic transitions from one to the other. The system size dependence of the transition frequency and dwell times shows a pronounced crossover that is determined by the ratio of the band width and the longitudinal system size. Our work paves the way for studying multispecies models with heterogeneous alignment interactions.

[1] T. Vicsek, A. Czirók, E. Ben-Jacob, I. Cohen, and O. Shochet, Phys. Rev. Lett. 75, 1226 (1995).

CPP 21.11 Tue 12:15 TOE 317

Two-potential model for molecular motors — •Sophie Klempahn and Helmut Schiessel — Cluster of Excellence Physics of Life, Technical University of Dresden, Germany

Molecular motors are highly efficient biological machines, which drive systems away from equilibrium and realise key biological processes. For the description of the molecular motor action, discrete jump processes as well as energy barriers with height differences can be used. However, these models are based on symmetric conditions or unidirectional motion and therefore do not capture real biological systems with fuel gradients or where the motion is not unidirectional. To predict the effect of molecular motors on the density distribution of cargo particles in one dimension, we introduce a two potential model. This model represents the cargo particles as active particles, in which the binding of molecular motors to the cargo particle causes the active part of motion. Furthermore, we use two different energy landscapes for jumps to the left or right side, to include motors moving back- and forward, asymmetric environment or two different molecular motors acting on the same cargo particle in different directions. The solution of a master equation with different energy landscapes for jumps to the left and right side results in specific extremal points in the probability density of the cargo particles and shows a ratchet effect in case of periodic potentials.

CPP 22: 2D Materials III (joint session HL/CPP)

Time: Tuesday 9:30–12:15 Location: POT 81

CPP 22.1 Tue 9:30 POT 81

Sub-THz detection in two dimensional systems and CVD graphene heterostructures — Franziska Linss[1], Vincent Strenzke[1], Pai Zhao[1], Chithra S. Sharma[1], Lars Tiemann[1], •Qin Hua[2], and Robert H. Blick[1] — [1]Center for Hybrid Nanostructures, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Suzhou Institute of Nanotech and Nanobionics (SINANO) of the Chinese Academy of Sciences (CAS), China

Electromagnetic radiation in the THz range can induce surface plasmons, i.e., a collective motion of electrons, in graphene-based devices. We fabricated a field-effect-transistor with asymmetric dual-grating gates (ADGG) to detect sub-THz radiation using large-scale graphene that was synthesized by chemical vapor deposition (CVD). The CVD graphene sheet is encapsulated between two flakes of hBN and placed on a highly doped Si wafer that acts as a back gate. The ADGG was structured on the top hBN flake. The control of the carrier concentration via electrostatic gates is crucial to match the resonance condition of the plasmons. The sample was characterized by sweeping the top gate voltage from -1 V to 2 V and the charge neutrality point was reached at a top gate voltage of 0.87 V at 4.2 Kelvin. Furthermore, we used a high electron mobility transistor (HEMT) to detect THz radiation, where the detection mechanism is based on a mixing with a reference radiation in a nonlinear medium. In this device, we can demonstrate sub-THz radiation at room temperature.

CPP 22.2 Tue 9:45 POT 81

Theory of non-local Andreev reflection through Andreev molecular states in graphene Josephson junctions — •Andor Kormányos[1], Eduárd Zsurka[1], Noel Plaszkó[1], and Péter Rakyta[1,2] — [1]Department of Physics of Complex Systems, Eotvos Lorand University, Budapest, Hungary — [2]Wigner Research Center for Physics, 29-33 Konkoly-Thege Miklos Str., H-1121 Budapest, Hungary

We propose that a device composed of two vertically stacked monolayer graphene Josephson junctions can be used for Cooper pair splitting. The hybridization of the Andreev bound states of the two Josephson junction can facilitate non-local transport in this normal-superconductor hybrid structure, which we study by calculating the non-local differential conductance. Assuming that one of the graphene layers is electron and the other is hole doped, we find that the non-local Andreev reflection can dominate the differential conductance of the system. Our setup does not require the precise control of junction length, doping, or superconducting phase difference, which could be an important advantage for experimental realization.

CPP 22.3 Tue 10:00 POT 81

Quantum Hall measurements near electric field controlled Lifshitz transitions in trigonally warped bilayer graphene — •Martin Statz, Anna Seiler, Jonas Pöhls, Moritz Knaak, Francesca Farlorsi, and Thomas Weitz — 1st Physical Institute, Faculty of Physics, University of Göttingen, Friedrich-Hund-Platz 1, Göttingen 37077, Germany

Various spontaneous symmetry broken phases such as Stoner ferromagnetism, spin-polarized superconductivity, a quantum anomalous Hall octet and a topologically non-trivial Wigner-Hall crystal phase have recently been reported in bilayer graphene (BLG) [1]. Since these interaction-driven phenomena are dictated by the ratio of the Coulomb and kinetic energy of carriers, they can be promoted by the formation of flat bands and a divergent density of states (DoS) near Lifshitz transitions (LT). Trigonally warped BLG at low vertical displacement fields (D-field) and carrier densities ($\sim 10^{11}$ cm^{-2}) displays one centre and three off-centre Dirac cones in each valley, and therefore offers a rich playground for correlated phases (CP) and changes in the Fermi surface topology by inducing charge density and D-field driven LT. Here, we report on quantum Hall measurements near charge density and D-field driven LT in trigonally warped BLG encapsulated in hexagonal boron-nitride in a dual-gated architecture with graphite contacts and graphite gates at 10 mK. We further outline our status on the temperature dependence of several CP in the aforementioned regimes.

[1] Seiler, A.M. et al. Nature 608, 298-302 (2022)

CPP 22.4 Tue 10:15 POT 81

Tuning electronic properties of graphene with a transferred ultrathin Ga_2O_3 encapsulation — Matthew Gebert[1], •Semonti Bhattacharyya[2], Christopher Bounds[1], Nitu Syed[3,4], Torben Daeneke[4], and Michael S. Fuhrer[1] — [1]School of Physics and Astronomy, Monash University, Melbourne — [2]Leiden Institute of Physics, Leiden University, Leiden — [3]School of Physics, The University of Melbourne, Parkville, Melbourne — [4]School of Engineering, RMIT University, Melbourne

Although graphene holds immense potential for future electronics and spintronics, it is tricky to find a suitable large-area encapsulation layer for graphene that enhances its properties. In this talk, I will demonstrate a large-area passivation layer for graphene by mechanical transfer of ultrathin Ga_2O_3 synthesized on the surface of liquid Ga metal.[1]

Electrical measurements of millimetre-scale passivated and bare CVD graphene on SiO_2 substrate indicate that the passivated graphene maintains its high field effect mobility, desirable for applications. Surprisingly, the temperature-dependent resistivity is reduced in our passivated graphene over a range of temperatures below 230 K, due to the interplay of screening of the remote optical phonon modes of the SiO_2 by the high dielectric constant of Ga_2O_3, and the relatively high characteristic phonon frequencies of Ga_2O_3. Raman spectroscopy and electrical measurements indicate that Ga_2O_3 passivation also protects graphene from further processing such as plasma-enhanced atomic layer deposition of Al_2O_3.

1. Gebert, Bhattacharyya et al, Nano Lett, https://doi.org/10.1021/acs.nano

CPP 22.5 Tue 10:30 POT 81

Hopping transport in ultraclean dual graphite gated bilayer graphene — •David Alexander Darek Emmerich[1], Eike Thomas Icking[1,2], Philipp Schmidt[1,2], Frank Volmer[1,3], Kenji Watanabe[4], Takashi Taniguchi[5], Bernd Beschoten[1], and Christoph Stampfer[1,2] — [1]RWTH Aachen University, Germany — [2]Forschungszentrum Jülich, Germany — [3]AMO GmbH, Advanced Microelectronic Center Aachen (AMICA), Germany — [4]Research Center for Functional Material, Japan — [5]International Center for Materials Nanoarchitectonics, Japan

Bernal-stacked bilayer graphene (BLG) is a material that has a unique property: BLG is intrinsically a semimetal, but becomes a semiconductor under the applicaton of an out-of-plane displacement field. This controlled opening of a gate-tunable band gap makes it a promising material for realizing highly-tunable transistors and photodetectors. The limiting factor of BLG-based devices is disorder. Only by using graphitic bottom gates a true band insulating state was achieved in BLG, which exhibits a clean gap opening with faint signs of residual disorder. Using finite bias spectroscopy, we show that BLG devices with graphitic top and bottom gate electrodes exhibit extremely low disorder. We perform transport measurements down to the sub-Kelvin regime and analyse the temperature-dependent transport behaviour. For small displacement fields, where gap and disorder are expected to be of the same order of magnitude, the low-temperature hopping transport data are investigated concerning the dominant hopping mechanism.

15 min. break

CPP 22.6 Tue 11:00 POT 81

high responsivity monolayer MoS_2 photodetectors on cyclic olefin copolymer-passivated SiO_2 gate dielectric — •Emad Najafidehaghani[1], Sirri Batuhan Kalkan[2], Ziyang Gan[1], Jan Drewniok[2], Michael F Lichtenegger[2], Uwe Hübner[3], Alexander S Urban[2], Antony George[1], Bert Nickel[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Jena — [2]Ludwig Maximilian University of Munich, Faculty of Physics, Munich — [3]Leibniz Institute of Photonic Technology (IPHT), Jena

2D material-based photodetectors attracted significant research interest due to their high responsivity, flexibility and transparency. However, the trap states present at the surface of SiO_2 gate dielectrics diminishes the performance of 2D material-based photodetectors. To reduce the detrimental effect of SiO_2 surface traps, an ultrathin film (5 nm) of cyclic olefin copolymer (COC) layer is employed as a surface passivator. Due to the reduction of the interface trap density, the photoresponsivity of the MoS_2 devices on passivated SiO_2 is enhanced by four orders of magnitude compared to non-passivated MoS_2 devices. Under optimized conditions a record photoresponsivity of 3×10^7 A/W in combination with a short response time is observed. Our findings show that the ultrathin COC passivation of the gate dielectric enables to probe exciting properties of the atomically thin 2D semiconductors.

CPP 22.7 Tue 11:15 POT 81

Atomic layer deposition of horizontal and vertical MoS_2/WS_2 heterostructures — •Christian Tessarek, Tim Grieb, Andreas Rosenauer, and Martin Eickhoff — Institut für Festkörperphysik, Universität Bremen

Beyond the properties of single two-dimensional (2D) layers, heterostructures made of 2D transition metal dichalcogenides promise new properties based on moiré physics and interlayer excitons.

Vertical and horizontal MoS_2 and WS_2 heterostructures were grown by atomic layer deposition (ALD) and analyzed by Raman and photoluminescence spectroscopy. The influence of the the ALD growth sequence, i.e. MoS_2/WS_2 vs. WS_2/MoS_2, was investigated. Elemental distribution of Mo and W in a horizontal heterostructure was studied by high resolution transmission electron microscopy and energy-dispersive X-ray spectroscopy. Additional high temperature annealing was performed to improve the structural and optical properties of the layers.

CPP 22.8 Tue 11:30 POT 81

Fully automated platform for 2D material flake detection using real-time machine learning techniques — •Jan-Lucas Uslu, Taoufiq Ouaj, Bernd Beschoten, Lutz Waldecker, and Christoph Stampfer — JARA-FIT and 2nd Institute of Physics A, RWTH Aachen University, Aachen, Germany

As of today, most of fundamental experimental 2D material research is based on mechanically exfoliated flakes, finding suitable flakes for the fabrication of van der Waal heterostructures is time-consuming and time-critical part requiring expert knowledge and manpower.

In order to mitigate this problem, we demonstrate a simple and robust real time-capable algorithm based on Gaussian mixture models, a machine learning technique, to allow for a fast automated search of exfoliated flakes of different 2D materials in a single run with an automated microscope setup to analyze batches of exfoliated material.

The algorithm solves the task of automatically detecting various flakes on Si++/SiO2 wafer dices, allows to index the location and segmentation of each flake and provides metrices such as size, thickness and shape.

The algorithm is evaluated on more than 500.000 images of different 2D materials including graphene and multilayer graphene, hexagonal boron nitride, transition metal dichalcogenides and 2D magnets.

CPP 22.9 Tue 11:45 POT 81

CVD Growth of Hexagonal Boron Nitride on CMOS-compatible Substrates — •Max Franck[1], Jarek Dabrowski[1], Markus Andreas Schubert[1], Walter Batista Pessoa[2], Dominique Vignaud[2], Luc Henrard[3], Christian Wenger[1,4], and Mindaugas Lukosius[1] — [1]IHP - Leibniz-Institut für innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]University Lille, CNRS, Centrale Lille, JUNIA ISEN, University Polytechnique Hauts de France, UMR 8520-IEMN F-59000 Lille, France — [3]Department of Physics, Namur Institute of Structured Materials, University of Namur, Rue de Bruxelles 61, 5000 Namur, Belgium — [4]Semiconductor Materials, BTU Cottbus-Senftenberg, Platz der Deutschen Einheit 1, 03046 Cottbus, Germany

Hexagonal boron nitride (hBN) is a two-dimensional insulator with a range of promising applications, including DUV optoelectronics and protection layers for high-mobility graphene. Most commonly, high-quality hBN is grown via CVD on catalytic transistion metal substrates. However, the hBN films require transfer to CMOS-compatible substrates, which leaves residual metal contaminations at concentrations unacceptable for Si technology integration.[1] Therefore, growth of hBN thin films directly on CMOS-compatible substrates, such as Si, Ge or dielectrics, is desirable. We present recent results regarding CVD synthesis of well-oriented, few-layer hBN films on such substrates using borazine as a single-source precursor. Morphology and crystallline quality were characterized using XPS, AFM, Raman spectroscopy and TEM. [1] G. Lupina, J. Kitzmann, et al. ACS Nano 2015, 9, 4776-4785.

CPP 22.10 Tue 12:00 POT 81

Microwave plasma driven 2H-1T phase modulation of WSe2 for improving NO2 gas sensing performance — •Yu Duan[1,2], Sam Zhang[2], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Center for Advanced Thin Films and Devices, School of Materials and Energy, Southwest University, Chongqing, 400715, China

Transition metal dichalcogenides (TMDs) have been widely used in recent years for gas sensors. Herein, we constructed a simple microwave plasma device by modifying a home microwave oven for surface treatment of WSe2. A 1T/2H hybrid phase structure was constructed by phase modulation and Se vacancies were introduced to effectively enhance its gas sensing performance. The sample after 60 s of treatment exhibited high response (52.24%), fast response rate (49.8 s), short recovery time (14.9 mins), and outstanding stability and selectivity for 1 ppm NO2 at room temperature. In addition, molecular model of the microwave plasma-treated sample is proposed, leading to the intrinsic mechanism of its performance enhancement. It is demonstrated that microwave plasma treatment is a promising method to enhance the gas sensing performance of TMDs.

CPP 23: Optical Properties (joint session HL/CPP)

Time: Tuesday 9:30–13:00 Location: POT 112

CPP 23.1 Tue 9:30 POT 112

Can Ge and Si be optoelectronic materials: Hexagonal polytypes — •Martin Keller[1], Abderrezak Belabbes[1,2], Jürgen Furthmüller[1], Friedhelm Bechstedt[1], and Silvana Botti[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörpertheorie und -optik, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Department of Physics, Sultan Qaboos University, P.O. Box 36, PC 123, Muscat, Oman

The group IV elements silicon and germanium crystallize in cubic diamond structure under ambient conditions and feature indirect bandgaps. Therefore they cannot emit light efficiently and are not applicable in active optoelectronic devices. Under high pressure, however, as well as using different growth techniques, several Si and Ge polymorphs, including hexagonal polytypes, have been observed. Lonsdaleite Ge as well as Ge-rich hexagonal alloys have even been found to have a direct bandgap and strongly emit light with varying frequency. Thus hexagonal systems have become of great interest for potential optical emitters that may be integratable with CMOS technology. We have performed extensive ab initio studies of the energetic, structural, elastic and electronic properties as well as the strengths of some dipole transitions of the hexagonal Si and Ge polytypes 2H, 4H and 6H using Density Functional Theory and approximate quasiparticle treatments, and trends between the different geometries are analysed. The results for cubic and hexagonal Si and Ge agree excellently with existing experimental findings. The electronic structures point to promising optical properties.

CPP 23.2 Tue 9:45 POT 112

Many-body effects in the mid-infrared dielectric function of InSb from 80 to 800 K — Melissa Rivero Arias, Cesy Zamarripa, Jaden Love, Carlos Armenta, Carola Emminger, Sonam Yadav, and •Stefan Zollner — New Mexico State University, Las Cruces, NM, USA

We describe measurements of the mid-infrared dielectric function of bulk InSb near the direct band gap using Fourier-transform infrared spectroscopic ellipsometry from 80 to 800 K in an ultra-high vacuum cryostat. Indium antimonide is the zinc blende compound semiconductor with the smallest direct band gap (E_0=0.18 eV at 300 K) due to its heavy elements and the large resulting spin-orbit splitting and Darwin shifts. The band gap is extracted from the dielectric function by fitting with a parametric oscillator model. It decreases from 80 to 450 K following a Bose-Einstein model, then remains constant up to 550 K, and increases again at the highest temperatures. This is explained with a thermal Burstein-Moss shift: The onset of optical absorption increases as electron-hole pairs are thermally excited at the highest temperatures. The intrinsic carrier concentration determined from the Drude tail in the ellipsometry spectra agrees qualitatively with temperature-dependent Hall experiments and calculations based on degenerate Fermi-Dirac statistics.

CPP 23.3 Tue 10:00 POT 112

Polarized Raman scattering study of epitaxially grown GeSn layers with various Sn content — •Agnieszka Anna Corley-Wiciak[1], Omar Concepción[2], Marvin Hartwig Zoellner[1], Detlev Grützmacher[2], Dan Buca[2], Giovanni Capellini[1,3], and Davide Spirito[1] — [1]IHP Leibniz-Institut für innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]Peter Grünberg Institute 9 (PGI-9) and JARA-Fundamentals of Future Information Technologies — [3]Dipartimento di Scienze, Università Roma Tre, V.le G. Marconi 446, 00146 Roma, Italy

$\mathrm{Ge_{1-x}Sn_x}$ alloys are an excellent candidate for developing mid-infrared light sources integrated with CMOS technology. The challenges in the controlled growth with high crystal quality have highlighted the peculiarity of these alloys, which can be monitored by their vibrational properties. To this purpose, Raman spectroscopy is an effective experimental method to determine these properties, as this technique is non-destructive, contactless, fast, and locally resolved. We use Raman scattering with different polarization configurations to investigate $\mathrm{Ge_{1-x}Sn_x}$ ($0.05 \leq x \leq 0.14$) alloys grown by Chemical Vapour Deposition on Ge/Si virtual substrates. Measurements were performed in backscattering geometry with parallel and cross polarizations. In this way, we identify multiple components in the vibrational modes and how they deviate from simplified models. Our results will help to understand the fundamental properties of $\mathrm{Ge_{1-x}Sn_x}$ alloys to enable fast assessment for their applications in optoelectronic and thermoelectric.

CPP 23.4 Tue 10:15 POT 112

Eigenmodes and Polarization Structure of Coupled Elliptical Microcavities — •Johannes Düreth[1], Simon Betzold[1], Monika Emmerling[1], Antonina Bieganowska[2], Jürgen Ohmer[3], Utz Fischer[3], Sven Höfling[1], and Sebastian Klembt[1] — [1]Technische Physik, RCCM and Würzburg-Dresden Cluster of Excellence ct.qmat, University of Würzburg, Germany — [2]Faculty of Problems of Fundamental Technology, Department of Experimental Physics, Laboratory for Optical Spectroscopy of Nanostructures, Wroclaw, Poland — [3]Department of Biochemistry, University of Würzburg, Germany

Elliptical potentials give rise to a set of eigenmodes called Ince-Gaussian modes. Contrary to hemispherical potentials, the geometric shape leads to a mode splitting of the otherwise degenerate fundamental mode. Theoretically, this behaviour can be exploited to realize interesting topological phenomena like non-reciprocal transport, the non-hermitian skin-effect or engineer artificial gauge fields. On the way to an experimental implementation of such systems, the singular building blocks of these photonic potentials - single and coupled elliptical potentials - have to be experimentally studied.

Here we present an investigation of the mode splitting and polarisation in single elliptical microcavities, as well as an examination of the coupling between differently angled ellipses.

15 min. break

CPP 23.5 Tue 10:45 POT 112

Optical properties of $\mathbf{Ag_xCu_{1\text{-}x}I}$ alloy thin films — •E. Krüger[1], M. Seifert[2], V. Gottschalch[3], H. Krautscheid[3], C.S. Schnohr[1], S. Botti[2], M. Grundmann[1], and C. Sturm[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany — [2]Friedrich-Schiller-Universität Jena, Institut für Festkörpertheorie und Optik , Germany — [3]Universität Leipzig, Institut für Anorganische Chemie, Germany

Copper iodide (CuI) is a promising wide bandgap semiconductor for applications in transparent optoelectronic devices. In this context, the specific tuning of electrical and optical properties, which can potentially be achieved with ternary alloys such as $\mathrm{CuBr_xI_{1\text{-}x}}$ [1] and $\mathrm{Ag_xCu_{1\text{-}x}I}$ [2], is crucial for the development of novel CuI-based devices. In particular, $\mathrm{Ag_xCu_{1\text{-}x}I}$ is of great interest because the intrinsic conductivity changes from p-type to n-type with increasing Ag content.

Here we present the bandgap energy and spin-orbit splitting in $\mathrm{Ag_xCu_{1\text{-}x}I}$ alloys as a function of alloy composition and temperature, studied by a combination of experimental and computational methods. The non-linear bandgap dependence on Ag content can be described by a quadratic bowing parameter of 0.54 eV and is dominated by charge carrier redistribution effects in the presence of unequal element-specific bond lengths. The slight increase of the spin-orbit splitting from 640 meV for CuI to about 790 meV for AgI is discussed in terms of decreasing p-d hybridization of the valence bands at the Γ-point.

[1] N. Yamada et al., Adv. Funct. Mater. **30**, 2003096 (2020)

[2] A. Annadi and H. Gong, Appl. Mater. Today **20**, 100703 (2020)

CPP 23.6 Tue 11:00 POT 112

Multipole theory of optical spatial dispersion in crystals — •Óscar Pozo — Centro de Física de Materiales, Universidad del País Vasco, 20018 San Sebastián, Spain

Natural optical activity is the paradigmatic example of an effect originating in the weak spatial inhomogeneity of the electromagnetic field on the atomic scale. In molecules, such effects are well described by the multipole theory of electromagnetism, where the coupling to light is treated semiclassically beyond the electric-dipole approximation. That theory has two shortcomings: it is limited to bounded systems, and its building blocks - the multipole transition moments - are origin dependent. In this work, we recast the multipole theory in a translationally-invariant form that remains valid for periodic crystals. Working in the independent-particle approximation, we introduce 'intrinsic' multipole transition moments that are origin independent and transform covariantly under gauge transformations of the Bloch eigenstates. Electric-dipole transitions are given by the interbank Berry connection, while magnetic-dipole and electric-quadrupole transitions are described by matrix generalizations of the intrinsic magnetic moment and quantum metric. In addition to multipole-like terms, the response of crystals at first order in the wave vector of light contains band-dispersion terms that have no counterpart in molecular theories. The rotatory-strength sum rule for crystals is found to be equivalent to the topological constraint for a vanishing chiral magnetic effect in equilibrium, and the formalism is validated by numerical tight-binding calculations.

CPP 23.7 Tue 11:15 POT 112

Predicting bandgap in strain-engineered multinary III-V semiconductors — •Badal Mondal and Ralf Tonner-Zech — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, 04103 Leipzig, Germany

The tuning of the type and size of bandgaps of III-V semiconductors is a major goal for optoelectronic applications. Varying the relative composition of several III- or V-components in compound semiconductors is one of the major approaches here. Alternatively, straining the system can be used to modify the bandgaps. By combining these two approaches, bandgaps can be tuned over a wide range of values, and direct or indirect semiconductors can be designed. However, an optimal choice of composition and strain to a target bandgap requires complete material-specific composition, strain, and bandgap knowledge. Exploring the vast chemical space of all possible combinations of III- and V-elements with variation in composition and strain is experimentally not feasible. We thus developed a density-functional-theory-based predictive computational approach for such an exhaustive exploration. This enabled us to construct the 'bandgap phase diagram' [1] by mapping the bandgap in terms of its magnitude and nature over the whole composition-strain space. Further, we have developed efficient machine-learning models to accelerate such mapping. We will show the application to binary [2], ternary and quaternary material combinations and the possible impact on device design.

[1] https://bmondal94.github.io/Bandgap-Phase-Diagram , 2022

[2] https://arxiv.org/abs/2208.10596

CPP 23.8 Tue 11:30 POT 112

GeSn vertical p/n photodetectors formed by 2-step ion implantation — •Shuyu Wen[1,2], Saif Shaikh[1], Oliver Steuer[1], Yonder Berencen[1], Slawomir Prucnal[1], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [2]Institute of Semiconductors, Chinese Academy of Sciences, Bejing, China

Germanium (Ge) is a promising material in integrated circuit (IC) due to the high mobility of hole carrier and highly compatibility in the Si-base IC technology. However, the indirect band structure of Ge leads to the low radiative recombination efficiency, limiting the application in opto-electronics. Alloying Ge with Tin (Sn) is a promising method to obtain energy band modification even to a direct band. Here, high quality Ge0.97Sn0.03 and Ge0.955Sn0.045 alloy is obtained by CMOS-compatible ion implantation method. Tensile strain leads by Sn alloying and damage recovery after Flash annealing (FLA) are characterized by Raman and XRD measurements. A subsequently phosphors implantation is applied to obtain vertical pn photodetectors (PD). The device shows an extended spectral response comparing with commercial Ge PD. This work provides a new CMOS-compatible method to fabricate photodetectors in short-wave infrared.

15 min. break

CPP 23.9 Tue 12:00 POT 112

Interplay between strain, Sn content and temperature in GeSn-based optoelectronic devices — •Ignatii Zaitsev[1], Agnieszka A. Corley-Wiciak[1], Dan Buca[2], Omar Concepción[2], Michele Virgilio[3], Giovanni Capellini[1,4], Costanza L. Manganelli[1], and Davide Spirito[1] — [1]IHP - Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany — [2]PGI 9, Jülich, Germany — [3]Università di Pisa, Pisa, Italy — [4]Università Roma Tre, Roma, Italy

Several works have shown the subtle interplay between thermomechanical strain, Sn content and band occupation in optoelectronic devices based on CMOS-integratable group-IV materials (Ge, SiGe, SiGeSn). This is especially the case when temperature plays a key role, e.g. devices operating at cryogenic temperature or in presence of high power. Here we provide a theoretical-experimental approach combining 3D FEM calculations, Raman and photoluminescence spectroscopy to fully capture the influence of mechanical and thermomechanical features on the optical properties. We apply this method to strained GeSn microdisks, a device geometry aimed at laser in the MIR range. With the presented methods, we can develop a thorough guidelines for the assessment and design of integrated light emitters.

CPP 23.10 Tue 12:15 POT 112

Excitons in MoS_2 bilayers under pressure — •Jan-Hauke Graalmann[1], Paul Steeger[2], Robert Schmidt[2], Steffen Michaelis de Vasconcellos[2], Rudolf Bratschitsch[2], and Michael Rohlfing[1] — [1]Institute of Solid State Theory, University of Münster, 48149 Münster, Germany — [2]Institute of Physics, University of Münster, 48149 Münster, Germany

Theoretical and experimental studies have shown that the optical spectrum of the MoS_2 bilayer changes under pressure.

Our theoretical investigations are based on DFT, *GdW* and the Bethe-Salpeter equation. For the specific stress conditions of the experiment, our calculations show an effective shift of the excitation energies of the A exciton towards higher energies with increasing pressure. This behaviour can be explained with an approximately constant direct band gap at the K point while the binding energy decreases. Due to a growing valence band splitting for increasing pressures, the interlayer exciton shows a smaller shift. These results are substantiated by measurements using a piston type diamond anvil cell (DAC) to create pressures in the GPa range.

The reason for only small changes of the fundamental band gap is a significant influence of interlayer interaction. The effect of a decreasing gap by biaxial lateral shrinking of each single layer under an external pressure gets counterbalanced by the reduction of the interlayer distance. Furthermore, the real space distribution shows an increased interlayer character for the A and interlayer exciton under pressure.

CPP 23.11 Tue 12:30 POT 112

Optical properties of a vacancy-related complex in 4H-SiC — •Maximilian Schober[1], Nicolas Jungwirth[1], Takuma Kobayashi[2], Johannes A. F. Lehmeyer[2], Michael Krieger[2], Heiko B. Weber[2], and Michel Bockstedte[1] — [1]Institute for Theoretical Physics, Johannes Kepler University Linz, Austria — [2]Lst. f. Angewandte Physik, Friedrich-Alexander-University Erlangen-Nürnberg, Germany

SiC is host to multiple color centers, such as the silicon vacancy, the divancy, and the carbon antisite-vacancy complex, with relevant applications as qubits, single photon sources and in quantum metrology. Recently, the carbon di-vacancy-antisite complex was identified as an annealing product of vacancy related defects [1], and is expected to feature favorable properties for quantum technology. The presence of strongly localized silicon and carbon dangling bonds points to rich photo- and spin physics that has so far not been explored in detail. In this work we probe the basal and axial configurations of $V_CC_{Si}V_C$ for their electronic-, optical- and radiative properties using a theoretical framework of hybrid density functional and many body approaches. We obtain the principal transitions, as well as the associated static- and transition dipole moments of the relevant charge states. Our results suggest a tentative identification of the carbon di-vacancy-antisite with the temperature-stable (TS) center [2].

[1] E. M. Y. Lee *et al.*, Nat. Commun. 12, 63 (2021).
[2] M. Rühl, C. Ott, S. Götzinger, M. Krieger, H. B. Weber, Appl. Phys. Lett. 113, 122102 (2018).

CPP 23.12 Tue 12:45 POT 112

Defects or Dots – what semiconductor physics can bring into optical super-resolution imaging — •Philipp Kellner[1], Jana Sütterlin[1], Paul Konrad[2], Andreas Sperlich[2], and Christian Eggeling[1,3] — [1]Institut für angewandte Optik und Biophysik, FSU Jena, Philosophenweg 7, 07743 Jena — [2]Physikalisches Institut, Julius-Maximilians Universität Würzburg, Am Hubland, 97074 Würzburg — [3]Institut für physikalische Hochtechnologie, Albert-Einstein-Straße 9, 07745 Jena

Super-resolved optical microscopy is a widely used tool throughout the medicine and biology community. Mostly and routinely done with organic dyes super-resolution imaging has led to various insights into cell structures and diffusional dynamics. The fundamental problem occurring with organic dyes is their rather dim brightness and their lack of photostability paired with photo-toxicity. This presentation will shed light on novel semi-conductor-based chromophores, like NV-centers in diamond, defects in hBN and CdTe quantum dots, and their use in optical nanoscale sensing schemes like StED-imaging or fluorescence correlation microscopy.

CPP 24: Complex Fluids and Soft Matter I (joint session DY/CPP)

Time: Tuesday 10:00–13:00 Location: MOL 213

CPP 24.1 Tue 10:00 MOL 213

How are mobility and friction related in viscoelastic fluids? — •Juliana Caspers[1], Nikolas Ditz[2], Karthika Krishna Kumar[2], Felix Ginot[2], Clemens Bechinger[2], Matthias Fuchs[2], and Matthias Krüger[1] — [1]Institute for Theoretical Physics, Georg-August Universität Göttingen, 37073 Göttingen, Germany — [2]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

The motion of a colloidal probe in a viscoelastic fluid is described by friction or mobility, depending on whether the probe is moving with a velocity or feeling a force. While the Einstein relation describes an inverse relationship valid for Newtonian solvents, both concepts are generalized to time-dependent memory kernels in viscoelastic fluids. We theoretically and experimentally investigate their relation by considering two observables: the recoil after releasing a probe that was moved through the fluid and the equilibrium mean squared displacement (MSD). Applying concepts of linear response theory, we generalize Einstein's relation and thereby relate recoil and MSD, which both provide access to the mobility kernel. With increasing concentration, however, MSD and recoil show distinct behaviors, rooted in different behaviors of the two kernels. Using two theoretical models, a linear two-bath particle model and hard spheres treated by mode-coupling theory, we find a Volterra relation between the two kernels, explaining differing timescales in friction and mobility kernels under variation of concentration.

CPP 24.2 Tue 10:15 MOL 213

Can liquid-state theory predict jamming of hard particles? — •Carmine Anzivino[1], Mathias Casiulis[2], Amgad Moussa[3], Stefano Martiniani[2], and Alessio Zaccone[1] — [1]Department of Physics "A. Pontremoli", University of Milan, via Celoria 16, 20133 Milan, Italy — [2]Center for Soft Matter Research, Department of Physics, New York University, New York 10003, USA — [3]Syngenta AG, 4058 Basel, Switzerland

By generalizing the notion of maximally random jammed (MRJ) state [1,2] to that of MRJ-line, we show [3] that it is reasonable to assume the most random branch of jammed states to undergo crowding in a way qualitatively similar to an equilibrium liquid. We then prove that, for hard-sphere systems, liquid-state theories can be succesfully used to estimate the RCP density, when the latter is identified with the densest isostatic point, i. e. the densest among the MRJ states with z=6.

Our finding is further enforced by the analysis of polydisperse systems. Either in the case of bidisperse and polydisperse hard spheres our prediction of the RCP density is in very good agreement with simulations, for a large values of size ratios and polydispersity.

[1] S. Toquato, T. M. Truskett, and P. G. Debenedetti, Phys. Rev. Lett. 84, 2064 (2000). [2] S. Torquato and F. H. Stillinger, Reviews of Modern Physics 82, 2633 (2010). [3] C. Anzivino, M. Casiulis, T. Zhang, A. S. Moussa, S. Martiniani and A. Zaccone, "Estimating RCP as the densest isostatic packing in bidisperse and polydisperse hard spheres", manuscript submitted (2022).

CPP 24.3 Tue 10:30 MOL 213

2D crystals of squares and the tetraic phase — •Peter Keim — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

Squares (5 micron edge-length) were manufactured from a photo-resist using a 3D nanoprinter (nanoscribe GT). In aqueous solution, particles sediment by gravity to a thin cover slide where they form a mono-layer of Brownian particles. The curvature of the cover slide can be adjusted from convex to concave, which allows to vary the area-density of the mono-layer from 700 to 1500 particles in the field of view. For low densities, the squares are free to diffuse and form a 2D fluid while for high densities they form a quadratic crystal. In analogy to 2D-melting by topological defects with an intermediate hexatic phase for isotropic particles (KTHNY-theory and Nobel-price 2016), a four-folded bond-order correlation function is used to resolve a tetratic phase with quasi-long-range orientational order but short rang translational order.

CPP 24.4 Tue 10:45 MOL 213

Transient microrheology unveils the presence of two relaxation processes in viscoelastic fluids — •Félix Ginot[1], Juliana Caspers[2], Luis Frieder Reinalter[1], Karthika Krishna Kumar[1], Matthias Krüger[2], and Clemens Bechinger[1] — [1]Fachbereich Physiks Universität Konstanz, 78457 Konstanz, Germany — [2]Institute for Theoretical Physics, Georg-August Universität Göttingen, 37073 Göttingen, Germany

We experimentally investigate the transient dynamics of a colloidal probe particle in a viscoelastic fluid after the driving force acting on the probe is suddenly removed. In this situation, the probe exhibits a strong backward recoil, with two distinct timescales. While the first timescale naturally originates from the viscoelastic properties of the fluid, the second timescale arises from the coupling between the probe and the bath. These experimental observations are in excellent agreement with a microscopic model which considers the probe particle to be coupled to two bath particles via harmonic springs. Interestingly, this model exhibits two sets of eigenmodes corresponding to reciprocal and non-reciprocal force conditions, and which can be experimentally confirmed in our experiments. We expect our findings to be relevant under conditions where particles are exposed to non-steady shear forces as this is encountered e.g. in microfluidic sorting devices or the intermittent motion of motile bacteria within their natural viscoelastic surroundings.

15 min. break

CPP 24.5 Tue 11:15 MOL 213

Phason strain-free growth of quasicrystals based on purely local rules and without repair mechanism — Stefan Wolf[1], Michael Engel[2], and •Michael Schmiedeberg[1] — [1]Institute of Theoretical Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

We introduce a simple model for the growth of colloidal quasicrystals where new particles are sequentially added according to specific local rules to the system in three dimensions. Subsequent changes to the particles are not allowed, i.e., no phasonic rearrangements can occur once a particle has been placed into the system. Our findings demonstrate that the purely local energetic rules are sufficient to obtain complex long-ranged order. Thus, phasonic rearrangements or fluctuations might be important to facilitate the formation of almost perfect quasicrystals [1-3] but they are not indispensable.

[1] C.V. Achim, M. Schmiedeberg, and H. Löwen, Phys. Rev. Lett. 112, 255501 (2014).

[2] A. Gemeinhardt, M. Martinsons, and M. Schmiedeberg, Eur. Phys. J. E 41, 126 (2018).

[3] K. Nagao, T. Inuzuka, K. Nishimoto, and K. Edagawa, Phys. Rev. Lett. 115, 075501 (2015).

CPP 24.6 Tue 11:30 MOL 213

Magnus force on microscopic spinning objects moving through non-Markovian baths — Xin Cao[1], •Debankur Das[2], Niklas Windbacher[1], Felix Ginot[1], Matthias Kruger[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, University Konstanz, 78464 Konstanz, Germany — [2]Institut für Theoretische Physik, Universität Göttingen, 37077 Göttingen Germany

When a spinning object moves through a fluid or air, its direction of motion becomes deflected due to the Magnus force that is perpendicular both to the moving direction and the spinning axis. Since the Magnus effect is caused by inertial effects within the surrounding medium, it should vanish at micro scales where viscous forces dominate over inertia. Recent experiments have observed the phenomenon similar to Magnus effect when a spinning colloids and there aggregates are externally driven through a viscoelastic fluid. Even though the deflection force shows a similar dependence on the spinning and translating velocity of the particles as in case of Magnus forces, its sign is reversed. Here, we have developed a theory of such motions which doesnot rely on the inertial effects but caused explicitly by the memory effect of the viscoelastic fluid. To better elucidate our theory we corroborate our results with experiments. Our theory successfully captures the density relaxation timescales of the viscoelastic fluid. Further we proposed viable theoretical predictions which can be verified with further experiments.

CPP 24.7 Tue 11:45 MOL 213

Preferential alignment of colloidal dumbbells with recoil direction — •Karthika Krishna Kumar[1], Félix Ginot[1], Juliana Caspers[2], Matthias Krüger[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, Germany — [2]Institute for Theoretical Physics, Georg-August Universität Göttingen, Germany

Unlike Newtonian fluids, viscoelastic fluids can store and dissipate energy on much longer timescales leading to non-Markovian dynamics. Hence, probing viscoelastic fluids using colloidal particles reveal complex dynamics in microscopic lengthscales. A consequence of this is the recoil behavior of a colloidal particle after dragging it through a viscoelastic fluid. In this work, we use a pair of colloidal particles stuck together due to depletion interactions forming a dumbbell-shaped structure. This gives the advantage of resolving the orientational component in addition to the translational components of the particle motion. Surprisingly, we report that the axis of the dumbbell tends to align with the direction of the motion during a recoil. The amplitude of this orientational component follows a non-linear trend even in the regime where translational recoil amplitudes show a linear increase with shear velocity. This behavior can no longer be explained by the linear two-bath particle model which is able to explain the bi-exponential translational recoils. Furthermore, the amplitude of this re-orientation increases with the initial angle at which the dumbbell is dragged. This points to an asymmetric distribution of elastic energy between the two particles of the dumbbell which might cause this effect.

CPP 24.8 Tue 12:00 MOL 213

Entropic phase diagram of twisted convex particles — •Poshika Gandhi and Anja Kuhnhold — Institute of Physics, University of Freiburg, Germany

The field of liquid crystal simulations has, over the years, benefitted immensely from the study of purely entropy driven systems. Since Onsager's[1] predictions of the existence of a nematic phase in long rods, the list of known phases of hard rod-like particles has grown to include phases like smectics and cholesterics.

An important parameter in the formation of these phases is the particle shape anisotropy. By considering unusual particle shapes new phases can be discovered. Recently, Dussi and Dijkstra[2] showed the formation of stable chiral nematic phase in twisted polyhedral particles using only entropic interactions.

We used Monte Carlo NVT simulations to produce phase diagrams of a different class of twisted particles - convex triangular and rectangular prisms. The results show a host of previously undiscovered phases arising from the shape anisotropy parameters like twist angle and aspect ratios.

[1] Onsager, L., Ann. N. Y. Acad. Sci., 51, 627 (1949).

[2] Dussi, S., Dijkstra, M., Nat Commun. 7, 11175 (2016).

CPP 24.9 Tue 12:15 MOL 213

Optimizing the Structure of Acene Clusters — •Philipp Elsässer and Tanja Schilling — Institute of Physics, University of Freiburg, Germany

In the production of organic solar cells, neutral acene cluster beams are used to create thin films. The molecules in these clusters can be arranged in various ways. Most types of acene molecules are quasi two dimensional with one long axis - they prefer stacked or herring-bone structures. Additionally, the positions of the molecules in a cluster may vary. Thus, the exact way of how they arrange has a strong influence on the overall energy of the cluster.

We have investigated the structures of anthracene, tetracene, and pentacene clusters with up to 30 molecules. In order to find the configurations at the global minimum of the potential energy surface with respect to the positions of the atoms, we applied the Basin-Hopping Monte-Carlo (BH) algorithm to atoms described by the polymer-consistent force field - interface force field (PCFF-IFF). We studied for these cluster structures the relative stability between different sizes of clusters, as well as the accessibility of the global minimum at different temperatures.

CPP 24.10 Tue 12:30 MOL 213

Ergodicity breaking in overpacked colloidal hard spheres — •Hans Joachim Schöpe — Universität Tübingen, Institut für angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

The ergodic hypothesis is an essential prerequisite for the applicability of statistical mechanics in thermodynamic equilibrium. Direct experimental evidence of the validity of the ergodic hypothesis is extremely rare. Furthermore, the question arises to what extent - if at all - ergodicity exists in non-equilibrium. We have realized a novel dynamic light scattering experiment, which makes it possible to determine the probability distribution of relaxation-times in colloidal suspensions. We present here a systematic study of the relaxation-time distribution in colloidal hard spheres at the transition from equilibrium to non-equilibrium. In thermodynamic equilibrium, we can impressively confirm the ergodic hypothesis and show that the fluctuations are of a Gaussian nature. Out of equilibrium, we can detect non-Gaussian behavior, which increases rapidly with increasing undercooling (overpacking). The ergodic hypothesis is no longer fulfilled in non-equilibrium. Furthermore, we observe that the metastable fluid ages in the induction stage, the non-Gaussian fluctuations increase in the time before crystallization sets in. To what extent these fluctuations cause crystallization must be clarified in the future.

CPP 24.11 Tue 12:45 MOL 213

Coacervates from a polyelectrolye and a small polyion: preparation, phase behavior and theoretical modeling — Lucy Coria-Oriundo[1], Eugenia Apuzzo[2], Santiago Herrera[1], Marcelo Ceolín[2], Gabriel Debais[1], Fernando Battaglini[1], and •Mario Tagliazucchi[1] — [1]Universidad de Buenos Aires, Bs.As., Argentina — [2]Universidad Nacional de la Plata, Bs.As., Argentina.

A mixture of oppositely charged polyelectrolytes, under the proper experimental conditions, can undergo liquid-liquid phase separation. The resulting polymer-rich phase is usually known as polyelectrolyte coacervate. This work reports liquid coacervates composed of a small polyanion (ferricyanide) and branched poly(ethyleneimine) (BPEI), a polycation. The phase diagram of the system was measured as a function of the concentration of both components at fixed pH = 6 and a concentration of added NaCl of 0.5 M. The salt resistance of the coacervate was studied and it was found that the coacervate is stable up to [NaCl] = 1.35 M. The phase diagram and salt-resistance experiments were modeled with a statistical-thermodynamics formalism that models the association of the oppositely charged species as a pseudo-chemical-equilibrium. The model fits very well the experimental data and was used to analyze the differences between polymer-polymer and polymer-small ion coacervates. Finally, the diffusion coefficient of ferricyanide within the coacervated (measured with cyclic voltammetry) was shown to increase 10 times when the concentration of added NaCl was increased from 0 to 1.2 M.

CPP 25: Molecular Electronics and Photonics (joint session TT/CPP)

Time: Tuesday 12:00–13:00 Location: HSZ 201

CPP 25.1 Tue 12:00 HSZ 201

Single photon emitters in hBN via ultra-low energy helium ion implantation — •Renu Rani[1], Mihn Bui[1,2], Chenfeng Lu[1,2], Bilal Malik[1,2], Felix Junge[3], Thorsten Brazda[1], Detlev Grützmacher[1,2], Hans Höfsäss[3], and Beata Kardynał[1,2] — [1]Peter Grünberg Institut-9, Forschungszentrum Jülich, Jülich — [2]Department of Physics, RWTH Aachen, Aachen — [3]II. Institute of Physics, University of Göttingen, 37077 Göttingen

A discovery of quantum emitters in hexagonal boron nitride (hBN) has recently incited immense interest for quantum technologies. It offers a platform for fundamental science but is also of interest for applications in quantum photonics owing to its robust single photon emission at room temperature. Recent studies have suggested that these SPEs are associated with intrinsic defects, which led to efforts to engineer the SPE in hBN by various methods such as plasma treatment, annealing, laser, e-beam and ion irradiation methods. Despite these efforts, the origin of single photon emission and the correlation of emission with particular defects still need to be scrutinized. Here we use ultra-low energy ion implantation to introduce defects in hBN. We show that helium ions with energies as low as 50 eV are extremely efficient in introducing single photon emitters in hBN. We also show that low temperature annealing increases the density of the emitters. We consider the possible defects that helium ions at the implantation energy can generate in hBN and use statistical data on single photon emitters to discuss the possible origin of the emission. Finally, we discuss the viability of creating emitters in pre-selected locations.

CPP 25.2 Tue 12:15 HSZ 201

Mechanosensitive single-molecule junctions — •Fabian Pauly — University of Augsburg, Augsburg, Germany

Quantum interference of electron waves passing through a single-molecule junction provides a powerful way to influence its electrical properties. By distorting a molecule, showing a destructive quantum interference, small changes of electrode distance can lead to huge changes of electrical conductance. This mechanosensitivity is a desirable feature for highly sensitive stress sensors. Here, I will discuss recent combined experimental and theoretical studies of mechanosensitive molecular wires based on paracyclophanes and porphyrins [1-4]. Experimental findings are interpreted in terms of quantum interference effects between molecular frontier orbitals by theoretical calculations based on density functional theory and the Landauer scattering formalism.

[1] D. Stefani et al., Nano Lett. 18, 5981 (2018)
[2] K. Reznikova et al., J. Am. Chem. Soc. 143, 13944 (2021)
[3] W. M. Schosser et al., Nanoscale 14, 984 (2022)
[4] C. Hsu et al., Chem. Sci. 13, 8017 (2022)

CPP 25.3 Tue 12:30 HSZ 201

Designing mechanosensitive molecules: A genetic algorithm-based approach — •Matthias Blaschke and Fabian Pauly — Institute of Physics, University of Augsburg, D-86159 Augsburg, Germany

Single molecules can be used as miniaturized functional electronic components, when connected to metallic electrodes. Mechanosensitivity describes a change of conductance for a certain change of electrode separation and is a desirable feature for applications such as ultrasensitive stress sensors [1-4]. We combine methods of artificial intelligence with high-level simulations based on electronic structure theory to design optimized mechanosensitive molecules from predefined building blocks. In this way we overcome time-consuming, inefficient trial and error cycles in molecular design. We unveil the black-box machinery usually connected to methods of artificial intelligence by presenting all important evolutionary processes. In addition, we identify general features that characterize well-performing molecules. Our genetic algorithm provides a systematic and powerful way to search chemical space and to identify the most promising molecular candidates.

[1] D. Stefani et al., Nano Lett. 18, 5981 (2018)
[2] K. Reznikova et al., J. Am. Chem. Soc. 143, 13944 (2021)
[3] W. M. Schosser et al., Nanoscale 14, 984 (2022)
[4] C. Hsu et al., Chem. Sci. 13, 8017 (2022)

CPP 25.4 Tue 12:45 HSZ 201

Towards cavity-mediated molecule-molecule coupling — •André Pscherer[1], Jahangir Nobakht[1], Tobias Utikal[1], Stephan Götzinger[2,1,3], and Vahid Sandoghdar[1,2] — [1]Max Planck Institute for the Science of Light, Erlangen, Germany — [2]Department of Physics, Friedrich- Alexander University Erlangen-Nürnberg (FAU), Erlangen, Germany — [3]Graduate School in Advanced Optical Technologies (SAOT), Friedrich-Alexander University Erlangen-Nürnberg, Erlangen, Germany

We recently demonstrated that a single molecule coupled to a Fabry-Pérot cavity reacts nonlinearly to light at the single-photon level. This was shown in four-wave mixing, optical switching and photon number sorting experiments [1]. We aim to exploit this level of control to couple two molecules to each other via the cavity mode and to explore two-photon transitions that become possible in such a system. We gain access to the excited state population through spectrally tailored cavity mirrors which transmit red-shifted fluorescence. In this contribution, we will report on our progress, challenges, and intermediate results.

[1] A. Pscherer et al., Phys. Rev. Lett. **127**, 133603 (2021)

CPP 26: Electrical, Dielectrical and Optical Properties of Thin Films

Time: Tuesday 14:00–14:45 Location: MER 02

CPP 26.1 Tue 14:00 MER 02

Electronic and optical properties of thin film P3HT-based thermoelectrics — •Simon Schraad[1,2], Benedikt Sochor[1], Constantin Harder[1,3], Peter Müller-Buschbaum[3,4], Tim Laarmann[1,2], and Stephan Volkher Roth[1,5] — [1]Deutsches Elektronen Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — [2]University Hamburg, Mittelweg 177, 20148 Hamburg, Germany — [3]MLZ, TUM, 85747 Garching, Germany — [4]Research Neutron Source Heinz Maier-Leibnitz, Lichtenbergstraße 1, 85747 Garching, Germany — [5]KTH Royal Institute of Technology, Teknikringen 56-58, Stockholm, Sweden

The polymer Poly(3-hexylthiophen-2,5-diyl) (P3HT) is widely considered in research of organic electronics. If doped with metal chlorides or nanoparticles, P3HT shows thermoelectric properties. Deposition of small gold domains inside the polymer films optimizes the charge transport properties and thermoelectric Seebeck-coefficient and hence the so-called figure of merit zT. There is usually an AU, P3HT intermixing layer near the surface, but implanting the dopant deep inside the organic films results in higher thermoelectric coefficients. P3HT and Poly(3-hexylthiophen-2,5-diyl)-block-poly(methyl methacrylate) (P3HT-b-PMMA) diblock copolymer derivates were prepared by spray deposition and doped via chloroauric acid. Here, structural, optical and (thermo-)electrical properties were determined using AFM, ellipsometry as well as conductivity measurements. The results are a first step towards sprayed organic thermoelectric device, with great scalability potential in future industrial applications.

CPP 26.2 Tue 14:15 MER 02

On the way to sustainable photoluminescent tags — •Heidi Thomas, Shuaifei Zhu, Sebastian Schellhammer, and Sebastian Reineke — IAPP, TU Dresden

Recently, by using amorphous purely organic systems, we have been able to develop transparent programmable luminescent tags (PLTs) which can be used for labelling application or data storage [1,2]. So far the system consists of a phosphorescent organic emitter embedded in poly(methyl methacrylate) on quartz substrate or flexible foil. An oxygen-blocking layer allows for the spatial control of the phosphoresence of the system. The demand for sustainable solutions is high motivating the design of ecofriendly information storage. Here we present the investigation of suitable biocompatible and/or biodegradable polymers and emitters for their use in PLTs.

[1] Gmelch, M.; Thomas, H.; Fries, F.; Reineke, S. Programmable Transparent Organic Luminescent Tags. Sci. Adv. (2019).

[2] Gmelch, M.; Achenbach, T.; Tomkeviciene, A.; Reineke, S. High-Speed and Continuous-Wave Programmable Luminescent Tags Based on Exclusive Room Temperature Phosphorescence (RTP). Adv. Sci. (2021).

CPP 26.3 Tue 14:30 MER 02

Programmed Assembly of Dipolar Precursors into Porous, Crystalline Molecular Thin Films — •Alexei Nefedov[1], Ritesh Haldar[1], Zhiyun Xu[1], Hannes Kühner[1], Dennis Hofmann[2], David Goll[2], Benedikt Sapotta[1], Stefan Hecht[3], Marjan Krstić[1], Carsten Rockstuhl[1], Wolfgang Wenzel[1], Stefan Bräse[1], Petra Tegerer[2], Egbert Zojer[4], and Christof Wöll[1] — [1]Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [2]Universität Heidelberg, Heidelberg, Germany — [3]RWTH Aachen University, Aachen, Germany — [4]Graz University of Technology, Graz, Austria

Liquid-phase, quasi-epitaxial growth has been used to stack asymmetric, dipolar organic compounds on inorganic substrates, permitting porous, crystalline molecular materials which lack inversion symmetry. This allows material fabrication with built-in electric fields. We describe a new programmed assembly strategy based on metal-organic frameworks (MOFs) that facilitates crystalline, non-centrosymmetric space groups for achiral compounds. Electric fields are integrated into crystalline, porous thin films with an orientation normal to the substrate. Changes in electrostatic potential are detected via core-level shifts of marker atoms on the MOF thin films and agree with theoretical results. The integration of built-in electric fields into molecular solids creates possibilities for band structure engineering to control the alignment of electronic levels in organic molecules and it may also be used to tune the transfer of charges from donors loaded via programmed assembly into MOF pores.

CPP 27: Glasses and Glass Transition I (joint session DY/CPP)

Time: Tuesday 14:00–15:00 Location: ZEU 147

CPP 27.1 Tue 14:00 ZEU 147

Dynamical phase transitions in trap models and universality classes of aging — •Diego Tapias[1] and Peter Sollich[1,2] — [1]Institute for Theoretical Physics, University of Göttingen, Germany — [2]Department of Mathematics, King's College London, London, UK

We investigate how aging and driving by trajectory biasing interact in two mean field models of glassy dynamics, widely known as trap models. We show that similarly to kinetically constrained models, the equilibrium state of the unbiased system above the glass transition temperature is located at the coexistence of two dynamical phases (active and inactive). In contrast, below this temperature, we find two different nonequilibrium scenarios: energetic (or activated) aging that is destroyed by any dynamical bias towards low activity, which we call "fragile aging", and entropic aging that is stable against the existence of such a dynamical bias, which we refer to as "robust aging". We conjecture that these categories have broader relevance as universality classes for aging dynamics in glassy systems.

CPP 27.2 Tue 14:15 ZEU 147

Fragile to strong crossover as general glassy feature — •Anshul Deep Singh Parmar and Andreas Heuer — Institute of Physical Chemistry, University of Münster, Corrensstrasse 28/30, 48149 Münster, Germany

As a liquid is cooled below the melting temperature, the dynamics become increasingly sluggish with the degree of supercooling, known as fragility. The fundamental question is whether the liquid ceases to flow at some finite temperature, the material undergoing the glass transition, or dynamics diverge smoothly to zero temperature. This is a central question of pivotal importance for unraveling the nature of glass and theoretical understanding, concealing with astronomical long observation times.

We circumvent this infeasibility by taking advantage of swap Monte Carlo with multi-billion speedups for equilibration well beyond the glass transition. Our investigation of a wide range of system sizes and temperatures across the experimental glass transition unveils the nature of the energy landscape. We observe a notable deviation from the Gaussian nature of the potential-energy landscape. Rapid depletion of states is associated with the glassy bottom of the landscape, unveiling the fragile to strong crossover is the general glassy behavior. Our result ultimately rules out the finite-temperature divergence and establishes the conceptualized Arrhenius description of the dynamics at low temperatures. Our findings are critical in advancing the investigation of glass in an experimental and theoretical framework.

CPP 27.3 Tue 14:30 ZEU 147

A solution to the plasticity of glasses based on topological physics — •Alessio Zaccone — Department of Physics, University of Milan, 20133 Milano, Italy

I will start by reviewing the microscopic theory of linear elasticity in amorphous solids which, from first-principles consideration of non-centrosymmetry in the particle contact environment, leads to mathematical predictions of elastic moduli in quantitative parameter-free agreement with numerical simulations of random jammed packings [1]. This theory fully accounts for the extra non-affine displacements which arise due to the lack of centrosymmetry in disordered solids. I will then show that non-affinity of particle motions gives rise to well-defined topological defects (dislocation-like topological defects, DTDs) which have recently been discovered in the displacement field of glasses [1] and later confirmed in [2]. The norm of the associated Burgers vector of these defects can be used as an accurate predictor of the onset of plastic flow and yielding of glasses, and, in combination with Schmid's law, it can explain the phenomenon of shear banding via self-organization of DTDs in slip systems at 45 degrees with respect to flow direction [4]. Broader implications of a unifying topological field theory of liquids and the glass transition will also be mentioned. [1] A. Zaccone and E. Scossa-Romano, Phys. Rev. B 83, 184205 (2011) [2] Z. W. Wu, Y. Chen, W.-H. Wang, W. Kob, L. Xu, arXiv:2209.02937 (2022)

CPP 27.4 Tue 14:45 ZEU 147

Confinement induced relaxations and phase behavior of a nanoconfined ionic liquid crystal — •Mohamed Aejaz Kolmangadi[1], Andreas Schönhals[1], Li Zhuoqing[2], and Patrick Huber[2] — [1]Bundesantalt für Materialforschung und -prüfung (BAM), Berlin, Germany — [2]Technical Univeristy Hamburg TUHH and DESY

We investigate the molecular dynamics and electrical conductivity of a linear shaped guanidinium based ILC confined in self-ordered nano porous alumina oxide membranes of pore size ranging from 180nm down to 25nm by employing broadband dielectric spectroscopy (BDS) and calorimetry. Calorimetric investigation reveals a complete suppression of the columnar - isotropic transition, while the plastic crystalline - columnar transition temperature decreases with inverse pore size and deviates from the Gibbs - Thomson equation. For the bulk case, BDS detects two relaxation modes in the crystalline phase, the gamma relaxation and the $\alpha 1$ relaxation, and two relaxation modes in the columnar phase, the $\alpha 2$ and $\alpha 3$ relaxation. For the confined case, all relaxation modes slow down compared to the bulk. However, for the least pore size (25 nm), the $\alpha 2$ relaxation is absent. We discuss the possible molecular origins of the different relaxation modes observed. For the bulk ILC, a clear jump of 4 orders of magnitude in the absolute values of DC conductivity occurs at the transition from the plastic crystalline to hexagonal columnar phase, for the confined ILC, this transition is smooth. DC conductivity is reduced for the confined case, except for the 25nm, where the values is similar to the bulk.

CPP 28: Molecular Electronics and Excited State Properties (joint session CPP/TT)

Time: Wednesday 9:30–12:30 Location: GÖR 226

CPP 28.1 Wed 9:30 GÖR 226

Strong Solvatochromism in a Two Metal Center Photocatalyst Molecule — •Miftahussurur Hamidi Putra[1] and Axel Gross[1,2] — [1]Universität Ulm Institut für Theoretische Chemie Mez-Starck-Haus Oberberghof 7 89081 Ulm Deutschland — [2]Helmholtz Institute Ulm (HIU) Electrochemical Energy Storage, 89069 Ulm, Deutschland

In the theoretical study presented here, we show that the electronic and optical properties of a molecular photocatalyst can strongly depend on the solvent it is dissolved in [1]. Ground-state density functional theory and linear response time dependent density functional theory calculations are applied in order to investigate the influence of implicit solvents on the structural, electronic and optical properties of a two metal center molecular photocatalyst $[(tbbpy)_2Ru(tpphz)PtI_2]^{2+}$ ($RuPtI_2$) [2]. These calculations predict a significant dependence of the HOMO-LUMO gap of the photocatalyst on the dielectric constant of the solvent. We elucidate the electronic origins of this strong solvatochromic effect and sketch the consequences of these insights for the use of photocatalysts in different environments.

[1] M. K. Nazeeruddin, S. M. Zakeeruddin, R. Humphry-Baker, M. Jirousek, P. Liska, N. Vlachopoulos, V. Shklover, C.-H. Fischer, M. Grätzel, Inorg. Chem. **38**, 6298-6305 (1999).

[2] M. G. Pfeffer, T. Kowacs, M. Wächtler, J. Guthmuller, B. Dietzek, J. G. Vos, S. Rau, Angew. Chem. **54**, 6627-6631 (2015).

CPP 28.2 Wed 9:45 GÖR 226

Dynamic Charge-Transport and Charge-Transfer Regimes for Electron-Phonon-Coupled Molecular Systems — •Michel Panhans, Sebastian Hutsch, and Frank Ortmann — Department of Chemistry, TU München

Different approaches for charge transport in organic solids exist but they differ significantly in the described physics of the electron-phonon coupling. In our recent work, we investigate the charge-transfer dynamics, the fading of transient localization (TL) and the formation of polarons for a large range of vibration frequencies and temperatures in the phase space of the two-site Holstein model. The combined numerical and analytical method is based on the time-domain Kubo formula of electrical conductivity to describe the highly correlated electron-phonon dynamics from femtoseconds to very large time scales, reaching nanoseconds. We identify three charge-transport regimes, which are TL, soft gating, and polaron transport. Of particular interest is the built up of correlations between the electronic motion and the nuclei manifesting in the crossover between TL and polaron transport. We find, that the transition between these two limiting cases is seamless at all temperatures and all adiabatic ratios even for the low-frequency vibrational modes that were often considered to be frozen.

CPP 28.3 Wed 10:00 GÖR 226

Multichromophore Macrocycles of Perylene Bisimide Dyes as Fluorescent OLED Emitters — •Björn Ewald[1], Ulrich Müller[1], Peter Spenst[2], Philipp Kagerer[1], Theodor Kaiser[1], Matthias Stolte[2], Frank Würthner[2], and Jens Pflaum[1] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]Institut für Organische Chemie and Center for Nanosystems Chemistry, University of Würzburg, 97074 Würzburg

Highly efficient electroluminescence from Organic Light Emitting Diodes (OLEDs) is limited by the non-radiative character of triplet states for conventional fluorophores. While fluorescent emitters benefit from high radiative recombination rates on the order of 10^9 s^{-1}, they lack from dark triplet states with lifetimes up to several μs or ms. Here we elucidate the potential of perylene bisimide macrocycles as a novel class of fluorescent OLED emitters by applying photon-correlation studies. The correlation experiments unfold additional excitonic relaxation pathways shortening the dark state lifetime for the covalently linked perylene bisimide chromophores. A trimeric chemical design leads to efficient single-photon emission from optically excited thin film samples and even under electrical operation in OLEDs. To the best of our knowledge this is the first indication of electrically-driven single-photon emission from a fluorescent molecule [1]. Therefor we consider our work to constitute an important step towards the design of state-of-the art fluorescent OLED emitters that might also feature a high potential for application in non-calssical single-photon sources.

[1] Ulrich Müller et al., Adv. Optical Mater. 2022, 10, 2200234.

CPP 28.4 Wed 10:15 GÖR 226

A Tool Kit for Analyzing Emission Spectra of Multi-Molecular States — •Sebastian Hammer[1,4], Theresa Linderl[2], Kristofer Tvingstedt[1], Wolfgang Bruetting[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [3]Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg — [4]Departments for Physics and Chemistry, McGill University, Montreal, Canada

The performance of opto-electronic devices is often crucially impacted by multi-molecular excited states such as charge-transfer (CT) states or excimers. Hence, the spectroscopic analysis of these states is a common tool in the characterization of such systems. Due to the many parameters at play full quantum mechanical interpretations are tedious and therefore the analysis is often performed on a phenomenological level only. Here we present a tool kit to analyze temperature dependent emission spectra using a Franck-Condon based approach with a single effective inter-molecular vibrational mode and discuss the implications of considering different potentials for the ground and excited state harmonic oscillators [1]. Finally, we show that fundamental parameters of the potential energy landscape can be extracted from temperature dependent steady state emission spectra using the example of a tetraphenyldibenzoperiflanthene:C_{60} CT hetero-structure [2]. Funding from the DFG (Project 490894053) is greatfully acknowledged.

[1] Hammer et al., *Mater. Horiz.*. (2022). doi: 10.1039/D2MH00829G

[2] Linderl et al., *Phys. Rev. Appl.*. **13** 024061 (2020)

CPP 28.5 Wed 10:30 GÖR 226

Singlet Fission search in polyacene molecules in gas-phase and on rare-gas clusters using ab initio methods — •Selmane Ferchane and Michael Walter — Institute of Physics, University of Freiburg, Germany

Singlet fission (SF), is a spontaneous photo-excited splitting phenomenon. Where an organic chromophore dimer, converts its singlet exciton into a pair of triplet excitons. A great promise for future photon-to-current conversion of solar energy using organic materials with high efficiency. To get more insight into these processes of SF, we employed different ab initio theories and approaches in our investigation, namely, density functional theory (DFT), TD-DFT, MCTDH, and CASPT2/CASSCF. Since the spatial orientation is crucial to whether the molecule will go SF and the rate of it due to the orbital coupling of both molecules, based on recent studies. We calculate the most favorable orientation of the chromophores with the binding energies in the gas phase and adsorbed on Argon and Neon surfaces. Then we calculate the lowest-lying excited states that contribute to the singlet and triple transition plus the search for the possible conical intersection that crosses the surface potential energies.

CPP 28.6 Wed 10:45 GÖR 226

Template-Designed Organic Electronics — •Klaus Meerholz — Chemistry Department, University of Cologne, Greinstr. 4-6, 50939 Cologne, Germany

Worldwide, organic electronic devices such as OLEDs and solar cells have revolutionized the field of electronics; however, technological progress has been largely made by empirical research and development, while fundamental knowledge is often still incomplete.

This presentation will report results from the DFG-funded Research Training Group Template-Designed Organic Electronics addressing the question, how structural order influences the optoelectronic properties of pi-conjugated materials, and how these properties can be improved via the use of templates for the optimization of devices. Our approach spans all the way from the design of appropriate pi-conjugated molecular building blocks and surface-active templates, investigation of surfaces and interfaces by different spectroscopies, fabrication of optoelectronic devices, and finally theoretically modelling.

CPP 28.7 Wed 11:00 GÖR 226

Optically detected magnetic resonance of TADF OLED emitters — •Pascal Schady, Mona Löther, Fabian Binder, Vladimir

Dyakonov, and Andreas Sperlich — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Thermally activated delayed fluorescence (TADF) is an efficient triplet harvesting mechanism for organic light-emitting diodes (OLED). Molecular TADF Donor-Acceptor type emitters are limited by low reverse intersystem crossing (rISC) rates and broad spectra, making them less suitable for potential OLED devices. In contrast, so-called multiple resonance (MR) effect emitters, are very promising as they show narrowband emission, even for deep blue wavelengths. MR-TADF emitters consist mostly of planar and rigidly bound benzyl groups with boron and nitrogen substituents for HOMO and LUMO pinning. As a result, the exchange integral is small, therefore the energy gap between singlet and triplet states is low enough to efficiently populate emissive singlet states by up-converting long-lived triplet states via thermal excitation, even at room temperature. However, many MR-TADF materials, like the DABNA-series behave differently in solution or as a solid. We therefore are investigating the spin system of those emitters by optically detected magnetic resonance (ODMR) in order to shed light on spin-dependent efficiency limiting pathways and how to address them to improve future OLED devices.

15 min. break

CPP 28.8 Wed 11:30 GÖR 226

Influence of Fluorination on the Temperature Dependent Optical Transition in β- Phase ZnPc Single Crystals — •Lisa Schraut-May[1], Kilian Strauss[1], Sebastian Hammer[2], Kilian Frank[3], Bert Nickel[3], and Jens Pflaum[1] — [1]Experimental Physics VI, University of Würzburg — [2]Departments of Physics and Chemistry, McGill University, Montreal, Canada — [3]Department of Physics, LMU Munich

The possibility of fluorination renders zinc phthalocyanine (ZnPc) an excellent model system to study the interplay between molecular packing and opto-electronic properties [1]. Here, we conduct temperature as well as polarisation dependent photoluminescence (PL) studies on β-phase ZnPc single crystals with different degrees of fluorination to modify the microscopic packing and, thus, the interaction between the molecules. For plain ZnPc an exceptionally sharp PL peak can be observed at temperatures below 100 K, which can be attributed to a superradiant enhancement [2]. Since this coherent coupling between several molecules strongly depends on the intermolecular spacing, we show, that this phenomenon can be steered by the fluorination of the molecules involved. We interpret the resulting PL signal and its temperature dependence in combination with X-ray studies by a model based on coupled excitons whose coupling is affected by the spatial anisotropy of the thermal contraction of the crystal lattice.

We thank the Bavarian research network SolTech for financial support. [1] Rödel et al., J. Phys. Chem. C (2022) [2] Hestand et al., Chem. Rev. (2018)

CPP 28.9 Wed 11:45 GÖR 226

Charge Delocalization and Vibronic Couplings in Quadrupolar Squaraine Dyes — Daniel Timmer[1], Fulu Zheng[2], Moritz Gittinger[1], Thomas Quenzel[1], •Daniel C. Lünemann[1], Katrin Winte[1], Yu Zhang[3], Mohamed E. Madjet[2], Jennifer Zablocki[4], Arne Lützen[4], Jin-Hui Zhong[1], Antonietta De Sio[1], Thomas Frauenheim[2], Sergei Tretiak[3], and Christoph Lienau[1] — [1]University of Oldenburg, Germany — [2]University of Bremen, Germany — [3]Los Alamos National Laboratory, USA — [4]University of Bonn, Germany

Squaraines are prototypical quadrupolar charge-transfer chromophores. Their optical properties are often rationalized using an essential state model, predicting that optical transitions to the lowest excited state (S1) are one-photon allowed and to the next higher state (S2) are only two-photon-allowed and that vibronic coupling to high-frequency modes is greatly reduced. Here, we combine time-resolved spectroscopy techniques and quantum-chemical simulations to test and rationalize these predictions. We find the one-photon-allowed S1 and two-photon-allowed S2 states to be energetically well-separated. Also, we find small Huang-Rhys factors, especially for the high-frequency modes. The resulting concentration of the oscillator strength in a narrow spectral region around the S1 transition makes squaraines almost perfect optical two-level. Thus, these molecules and their aggregates are exceptionally interesting for e.g. strong coupling applications. [1]: Timmer, Daniel, et al., J. Am. Chem. Soc., 144, 41, 19150-19162 (2022)

CPP 28.10 Wed 12:00 GÖR 226

In-operando observation of polaron formation in SAMFETs using NEXAFS spectroscopy — Manuel Johnson, •Andreas Späth, Baolin Zhao, Marcus Halik, and Rainer H. Fink — FAU Erlangen-Nürnberg, Erlangen, Germany

We present an in-operando near-edge x-ray absorption fine structure (NEXAFS) study on p-type BTBT-based self-assembled monolayer (BTBT-SAM) films. As a 2D-model system, the BTBT-SAM offers direct electron spectroscopic insight into the active organic semiconductor layer without interfering bulk contributions. This optimized geometry allows for the first time the observation of polaronic states caused by charged species at the dielectric/organic interface using a core-level spectroscopic tool. Linear NEXAFS dichroism is employed to derive the molecular orientation of the BTBT subunit. In addition to the conventional C K-edge NEXAFS resonances, we observe modifications in the density of unoccupied states. The spectral changes are affected by the strength and polarity of the applied gate voltage. Furthermore, the related energies match the energy levels of polaronic states. Thus, we have clear indications to interprete the data in the context of polaron formation due to charge accumulation induced by the applied electric field in our ultrathin device.[1] The study has been funded by the DFG within GRK 1896 and the SolTECH initiative. [1] M. Johnson et al., Appl. Phys. Lett.121 (2022) 183503.

CPP 28.11 Wed 12:15 GÖR 226

Machine learning for molecular design of organic molecules and reaction optimization — •Julia Westermayr[1], Reinhard J. Maurer[2], and Detlev Belder[3] — [1]Artificial Intelligence in Theoretical Chemistry Group, Leipzig University, Germany — [2]Computational Surface Chemistry Group, University of Warwick, UK — [3]Analytical Chemistry, Leipzig University, Germany

High-throughput screening of reaction conditions and electronic properties of molecules plays a crucial role in chemical industry and can be facilitated by automated workflows and machine learning. However, the high combinatorial complexity of the various parameters affecting molecular properties leaves unguided searches in chemical space highly inefficient and the optimization of reactions to synthesize these molecules often fails as theoretical protocols are usually decoupled from experiments. In this talk, we will show how predictive and generative deep learning models can be combined to theoretically design new molecules with potential relevance to organic electronics [1]. Further, we will present how these tools can be coupled with experiments to enable automated micro-laboratories [2] for targeted chemical synthesis. [1] JW et al. Nat. Comp. Sci, in press (2023). [2] R. J. Beulig et al., Lab Chip 17, 1996 (2017).

CPP 29: Interfaces and Thin Films

Time: Wednesday 9:30–12:45 Location: MER 02

Invited Talk CPP 29.1 Wed 9:30 MER 02
Imaging mineral-water interfaces with atomic force microscopy — •Angelika Kühnle — Bielefeld University, Bielefeld, Germany

Mineral-water interfaces are omnipresent in nature and technology. Consequently, mineral-water interfaces play a decisive role in many fields, ranging from geochemistry, environmental science and biomineralization to catalysis and electrochemistry. A comprehensive understanding of the interaction of minerals with their surroundings requires the knowledge of the atomic surface structure including the hydration at the interface. In this respect, atomic force microscopy allows for gaining real-space, molecular-level information of the interfacial structure. In this presentation, silver iodide will be discussed as a prototypical example for an ice nucleating material. Silver iodide is a polar material, calling for a stabilization mechanism. So far, however, the stabilization mechanism is unknown. Our atomically resolved atomic force microscopy images reveal no indication for a surface reconstruction at the atomic scale, indicating that another mechanism seems to be at play.

CPP 29.2 Wed 10:00 MER 02
Template-Induced Growth of Sputter-Deposited Gold Nanoparticles on Ordered Porous TiO2 Thin Films for SERS Sensors — •Suzhe Liang[1], Tianfu Guan[1], Shanshan Yin[1], Eva Krois[2], Wei Chen[1], Christopher R. Everett[1], Jonas Drewes[3], Thomas Strunskus[3], Marc Gensch[1,4], Jan Rubeck[4], Christoph Haisch[2], Matthias Schwartzkopf[4], Franz Faupel[3], Stephan V. Roth[4,5], Ya-Jun Cheng[6], and Peter Müller-Buschbaum[1,7] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching — [2]TUM School of Natural Sciences, Chair of Analytical Chemistry and Water Chemistry, Garching — [3]LS Materialverbunde, Institut für Materialwissenschaft, CAU, Kiel — [4]DESY, Hamburg — [5]Department of Fibre and Polymer Technology, KTH, Stockholm, Sweden — [6]Ningbo Institute of Materials Technology & Engineering, CAS, Ningbo, China — [7]MLZ, TUM, Garching

Ordered porous gold/titanium dioxide (Au/TiO2) hybrid nanostructured films are specifically interesting in large-scale applications using localized surface plasmon resonances (LSPRs) and surface-enhanced Raman scattering (SERS). We investigate the optical response of sputter-deposited Au/TiO2 nanohybrid thin films with a focus on the plasmonic response and application as molecular sensors. To elucidate the origin of this behavior, we apply in situ grazing-incidence small-angle X-ray scattering (GISAXS) to investigate the growth kinetics of Au on a TiO2 template during sputter deposition. The Raman intensity of deposited molecules, probed with rhodamine 6G (R6G), depends on the deposited gold thickness.

CPP 29.3 Wed 10:15 MER 02
Proteins as stabilizers for foam films: Untangling the different stabilizing effects — •Kevin Gräff, Sebsatian Stock, Luca Mirau, Sabine Bürger, and Regine von Klitzing — Soft Matter at Interfaces, Technische Universität Darmstadt, Darmstadt, Germany

Macroscopic foams consist of foam films, which separate the single air bubbles from each other. Investigation of foam films is crucial to understand macroscopic foam properties such as foam stability. In order to untangle electrostatic, steric and network stabilization effects, we study and compare two globular proteins (β-lactoglobulin and bovine serum albumin) and a disordered, flexible protein (whole casein) at low ionic strengths with varying solution pH. Image intensity measurement allows to record spatially resolved disjoining pressure isotherms in a Thin Film Pressure Balance (TFPB). This reveals insights into the structure formation in inhomogeneous protein films. We introduce inhomogeneity tracking (feature-tracking) as a novel method to enable the measurement of interfacial mobility and stiffness of foam films. Around the isoelectric point, Newton Black Films form which are stable for the globular proteins while they are unstable for the disordered flexible one. This difference in film stability is explained by different characteristics of the network structures which is supported by findings in the bulk and at the surface of the respective protein solutions.

[1] Gräff, K. et al, (2022), Untangling effects of proteins as stabilizers for foam films, Front. Soft. Matter 2:1035377.

CPP 29.4 Wed 10:30 MER 02
Anomalous underscreening in concentrated aqueous electrolytes: myth or reality? — Saravana Kumar[1], Peter Cats[2], Igor Siretanu[1], René van Roij[2], and •Frieder Mugele[1] — [1]Physics of Complex Fluids, Univ. Twente, Enschede, The Netherlands — [2]Institute for Theoretical Physics, Utrecht Univ., Utrecht, The Netherlands

Recent surface forces apparatus experiments that measured the forces between two mica surfaces and a series of subsequent theoretical studies suggest the occurrence of universal underscreening in highly concentrated electrolyte solutions. We performed a set of systematic Atomic Force Spectroscopy measurements for aqueous salt solutions in a concentration range from 1 mM to 5 M using chloride salts of various alkali metals. Experiments were carried out using flat substrates and submicrometer-sized colloidal probes made of smooth oxidized silicon immersed in salt solutions at pH values of 6 and 9 and temperatures of 25degC and 45 degC. While strong repulsive forces were observed for the smallest tip-sample separations, none of the conditions explored displayed any indication of anomalous long range electrostatic forces as reported for mica surfaces. Instead, forces are universally dominated by attractive van der Waals interactions at tip-sample separations beyond approximately 2nm for salt concentrations of 1 M and higher. Complementary calculations based on classical density functional theory for the primitive model support these experimental observations and display a consistent decrease in screening length with increasing ion concentration.

CPP 29.5 Wed 10:45 MER 02
Layer-by-Layer Spray-deposition of Cellulose and Lignin — •Shouzheng Chen[1,2], Constantin Harder[1,3], Iuliana Ribca[4], Luciana Pluntke[1,5], Markus Oberthuer[5], Mats Johansson[4], Julien Navarro[2], and Stephan V. Roth[1,4] — [1]DESY, 22607 Hamburg, Germany — [2]University Hamburg, 20146 Hamburg, Germany — [3]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [4]KTH Royal Institute of Technology, 10044 Stockholm, Sweden — [5]HAW,Department Design, 22087 Hamburg, Germany

Cellulose and lignin are the main chemical components of wood and can be further processed and purified into more valuable chemical raw materials such as cellulose nanofibrils (CNF), Kraft lignin and lignosulfonate. Using the idea of a bottom-up approach, CNF-Lignin composite films were prepared by layer-by-layer (LbL) spray-deposition with CNF and different lignins. CNFs provide a three-dimensional porous network structure, and lignin molecules are attached to the structure of CNF to form a homogeneous structure. In addition, Kraft lignin and lignin derivatives contain a large number of phenolic hydroxyl groups, which might be preferential for thermoelectricity. Thus, CNF-Lignin composite film is an ideal template for composite functional materials.

CPP 29.6 Wed 11:00 MER 02
Growth Kinetics and Molecular Mobility of the adsorbed Layer of Poly(bisphenol-A Carbonate) (PBAC), Polysulfone (PSU), and Poly (2-Vinyl Pyridine) (P2VP) — •Hassan Omar, Paulina Szymoniak, Andreas Hertwig, and Andreas Schönhals — Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany

Interactions between a polymer and a substrate interface play a vital role in understanding the improvement in thin film material properties as well as serving as a model for nanocomposites. For any non-repulsive polymer-substrate interactions, polymer segments form an irreversibly adsorbed layer and show a slowdown in the glassy dynamics and thus an increase in the thermal glass transition temperature compared to the bulk-like values. The growth kinetics of the adsorbed layer obey a two-step mechanism: formation of immobilized layer with flat segmental conformations and a loosely bound layer with stretched chains pinned to the surface. Here the adsorbed layer was studied for: poly (bisphenol-A carbonate) (PBAC) and polysulfone (PSU), two bulky polymers containing a functional group (phenyl ring) in the backbone and compared to poly (2-vinyl pyridine) (P2VP), where the backbone is a vinyl-derivative and the functional group (pyridine) is in the side chain. The growth kinetics for PBAC and PSU were found to deviate from the well-known mechanism, observed for polymers such as

P2VP. Atomic force microscopy and ellipsometry were used for this investigation and was additionally supported by broadband dielectric spectroscopy.

15 min. break

CPP 29.7 Wed 11:30 MER 02

Influence of heavy chalcogen atoms on structural arrangement and spectroscopic properties in molecular donor/acceptor thin film heterostructures — •Elena Chulanova[1], Anton Pylypenko[1], Alexander Gerlach[1], Jannika Lauth[2], and Frank Schreiber[1] — [1]Institute for Applied Physics, University of Tübingen, 72076 Tübingen, Germany — [2]Institute for Physical and Theoretical Chemistry, University of Tübingen, 72076 Tübingen, Germany

Organic semiconductors are widely used in optoelectronics due to their tunable electronic and structural properties. For many applications, the active layers consist of heterostructures and the details of the interaction between an electron donating and accepting moieties are the key factors for enhancing devices' efficiency. The chalcogenadiazole ring is a common acceptor core for organic chromophores and a variety of its condensed derivatives is known and used in this context. The presence of heavy chalcogens in the latter can impact the spin-orbit coupling and affect the optical properties. Here, we present a study on organic binary mixtures in thin films prepared by vacuum deposition, namely of dibenzochalcogenadiazolopyrazines as acceptors and known donors; i.e. diindenoperylene, pentacene, α-sexithiophene. The bulk heterojunction geometry was used with two materials mixed on the molecular level. We discuss the correlation between the mixing behavior of the molecules, and their structural and optical properties to obtain a systematic understanding of the processes occurring in molecular D-A systems based on 1,2,5-chalcogenadiazoles.

CPP 29.8 Wed 11:45 MER 02

The influence of increased kinetic energy of gold deposition onto polymers — •Yusuf Bulut[1,2], Benedikt Sochor[1], Kristian Reck[3], Jonas Drewes[3], Suzhe Liang[2], Tianfu Guan[2], Thomas Strunskus[3], Franz Faupel[3], Peter Müller-Buschbaum[2,4], and Stephan V. Roth[1,5] — [1]DESY, 22607 Hamburg — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [3]CAU Kiel, Chair for Multicomponent Materials, Faculty of Engineering, 24143 Kiel — [4]MLZ, TUM, 85748 Garching — [5]KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, SE-100 44 Stockholm

High Power impulse magnetron sputtering (HIPIMS) is a novel industrial relevant deposition technique enabling thin metal layers being coated onto polymers with increased adhesion and density. Compared to conventional direct current magnetron sputtering, no pre- and post-treatment is required to achieve these properties. So far there is no report discussing the nucleation and growth process during HiPIMS deposition. In this study, the polymer templates polystyrene (PS), poly-4-vinylpyridin (P4VP) and polystyrene sulfonicacid (PSS) are studied. Even though the polymers are very similar in their structure, it is expected that the distinct different functional moiety influence the kinetics of the initial growth stages of the gold layer. Results of simultaneous in situ grazing-incidence small angle X-ray scattering (GISAXS) and grazing incidence wide angle X-ray scattering (GIWAXS) are presented.

CPP 29.9 Wed 12:00 MER 02

Analysis of non-equilibrium thin film growth using X-ray photon correlation spectroscopy — •Ingrid Dax[1], Ivan Zaluzhnyy[1], Michael Sprung[2], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Thin film growth is a classic example of a non-equilibrium process in which a wide variety of functional properties can be obtained depending on the growth kinetics. Understanding the microscopic dynamics underlying the growth of molecular materials is an essential prerequisite for the rational design of complex structures and morphologies with controlled properties.

We perform in-situ X-ray experiments in grazing incidence geometry to follow the formation of thin film growth in real time, which reveals details of the dynamics during this process. This includes the adsorption of molecules on the substrate and the subsequent formation, realignment and diffusion of resulting molecular islands.

Specifically, we use modern coherent techniques based on X-ray photon correlation spectroscopy (XPCS). This resolves dynamics on the scale of 50-1000 nm, providing an unprecedented level of detail into the growth and diffusion of molecular islands during the growth process. We decompose our measurements into dynamic and kinetic time scales by comparing them to simulations, and interpret the results using established XPCS tools. This allows us to show that the time scales of a few 100 seconds are mainly due to kinetics, i.e., the growth of the islands.

CPP 29.10 Wed 12:15 MER 02

In situ GISAXS investigation of sputtering IZO thin film for optoelectronic applications — •Huaying Zhong[1], Lukas V Spanier[1], Christopher R. Everett[1], Xinyu Jiang[1], Shanshan Yin[1], Marlene Sophie Härtel[2], Jiahuan Zhang[2], Bertwin Bilgrim Otto Seibertz[3], Matthias Schwartzkopf[4], Stephan V. Roth[4,5], and Peter Müller-Buschbaum[1,6] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]HZB, Solar Energy, Berlin, Germany — [3]Department of technology for thin-film components, TU Berlin, Berlin, Germany — [4]DESY, Hamburg, Germany — [5]Department of Fibre and Polymer Technology, KTH, Stockholm, Sweden — [6]MLZ, TUM, Garching, Germany

Transparent conducting oxide (TCO) thin films have been studied intensively for optoelectronic devices, such as photodetectors, photovoltaics and light emitting diodes (LEDs). Among the several TCO thin films, zinc doped indium oxide (IZO) has received much attention as interface layer in optoelectronic devices due to its excellent electrical conductivity, optical transmittance, high thermal/chemical stability, low cost and low deposition temperature. Here, ITO glass and spin coated ZnO on ITO glass are used as the templates for IZO thin film deposition via DC magnetron sputtering technique. The growth dynamics of IZO film on these two templates are respectively investigated via grazing small angle x-ray scattering (GISAXS) characterization, and the morphology and optoelectrical properties of final films are further investigated.

CPP 29.11 Wed 12:30 MER 02

Investigation of Mg(0001) and Mg(1010) surfaces in Grignard electrolytes by reflection anisotropy spectroscopy — •Mario Löw[1], Holger Euchner[2], and Matthias M. May[1,2] — [1]Universität Ulm, Institute of Theoretical Chemistry, 89081 Ulm, Germany — [2]Universität Tübingen, Institute of Physical and Theoretical Chemistry, 72076 Tübingen, Germany

The high abundance and large volumetric capacity of the metal anode make rechargeable magnesium batteries potential candidates for future battery technologies. While understanding and controlling the electrode-electrolyte interface is essential for battery performance, there is often little known about the underlying atomistic interface structure under operating conditions [1].

To address this issue for the case of Mg, we study single crystalline magnesium surfaces in contact with standard Grignard electrolytes and under applied potential [2]. We employ reflection anisotropy spectroscopy (RAS) as an optical, high-resolution technique for the operando investigation of the interfacial structure as a function of the applied electrode potential. The Mg-crystal surface is studied in various solvents and Grignard electrolytes during voltammetric cycling. Finally, we seek comparison to theoretical spectra obtained within the random phase approximation.

[1] Popovic, Jelena. Nature Communications 12.1 (2021): 1-5.

[2] Lu, Z., et al. Journal of Electroanalytical Chemistry 466.2 (1999): 203-217.

CPP 30: Biopolymers and Biomaterials I (joint session BP/CPP)

Time: Wednesday 9:30–13:00 Location: TOE 317

CPP 30.1 Wed 9:30 TOE 317

Interaction of laminin and brain cells with ion implanted titania nanotube scaffolds — •Jan Frenzel[1,2,3], Astrid Kupferer[1,2], and Stefan Mayr[1,2] — [1]Leibniz Institute of Surface Engineering (IOM), 04318 Leipzig, Germany — [2]Division of Surface Physics, Faculty of Physics and Earth Sciences, Leipzig University, 04103 Leipzig, Germanyany — [3]Research Group Biotechnology and Biomedicine, Faculty of Physics and Earth Sciences, Leipzig University, 04103 Leipzig, Germany

Brain-machine interfaces enable symptomatic treatment of neurodegenerative diseases by modulating neural activities and enjoy great popularity when brain tissue is assessed ex vivo. However, current-use interface materials are troubled by numerous challenges concerning loss of long-term adhesion, rejection reactions, and glial scarring. We show that ion-implanted titania nanotube scaffolds (TNS) are a promising candidate for dealing with these issues because they combine high biocompatibility with adequate electrical conductivity. Based on our experiments, we explain how changes in the adsorption of laminin and the viability/adhesion of neurons and glial cells caused by ion implantation can be described by alterations in surface characterisics. The high neuron viability observed on all TNS, but suppressed glial cell formation on implanted TNS, demonstrates the potential as a future interface material. We acknowledge funding by SMWK (100331694). Reference: Frenzel et al., Nanomaterials 2022, 12, 3858. https://doi.org/10.3390/nano12213858

CPP 30.2 Wed 9:45 TOE 317

Fiber-based femtosecond 3D printing — •Claudia Imiolczyk[1], Andy Steinmann[1], Moritz Flöss[1], Zhen Wang[1], Michael Heymann[2], Andrea Toulouse[3], and Harald Giessen[1] — [1]4th Physics Institute, Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Institute of Biomaterials and Biomolecular Systems, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [3]Institute of Applied Optics, Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart, Germany

Ultrashort laser pulses are often used in medical applications, for instance for soft-tissue surgeries. However, the progress on using such laser pulses for tissue structuring is rather marginal so far. Therefore, we aim to realize an endoscopic fiber-based femtosecond 3D printer to minimally invasively surgically repair organ damage on a micrometer scale. For this, high-power femtosecond laser pulses are required, in order to 3D print desired geometries with a microfluidic bio-ink using two-photon-lithography. We utilize ruled reflective diffraction gratings to pre-chirp laser pulses, as dispersion in optical fibers broadens these femtosecond laser pulses. We report on measurements of pulse duration, spectrum, compression, and nonlinear effects. These resulting 3D printed structures should be colonized with endogenous cells, analogous to the extracellular matrix. This could open a new area of endoscopic 3D printing of biomaterials inside the human body to revolutionize plastic micro-surgery, such as repairing defects in the heart of embryos or even repairs behind the eardrum at the auditory ossicles.

CPP 30.3 Wed 10:00 TOE 317

DNA-encoded viscoelastic matrices for cell and organoid culture — •Elisha Krieg — Leibniz-Institut für Polymerforschung Dresden e.V. — Technische Universität Dresden

The recent advances in mechanobiology and the physics of life have driven an immense interest in mechanically programmable viscoelastic materials for cell and organoid culture. Here I describe a class of soft hydrogels based on novel DNA libraries that self-assemble with synthetic polymers.[1] This dynamic DNA-based matrix (DyNAtrix) provides computationally predictable, systematic, and independent control over key cell-instructive properties by merely changing DNA sequence information without affecting the compositional features of the system. This approach enables: (1) thermodynamic and kinetic control over network formation; (2) adjustable heat activation for the homogeneous embedding of mammalian cells; and (3) dynamic tuning of stress relaxation times to precisely recapitulate the mechanical characteristics of living tissues. DyNAtrix is self-healing, printable, exhibits high stability, cyto- and hemocompatibility, and controllable degradation. DyNAtrix-based 3D cultures of human mesenchymal stromal cells, pluripotent stem cells, canine kidney cysts, and placental organoids exhibit high viability, proliferation, and morphogenesis over several days to weeks. DyNAtrix thus represents a programmable and versatile precision matrix, paving the way for advanced approaches to biomechanics, biophysics, and tissue engineering.

[1] Peng et al. bioRxiv 2022, DOI:10.1101/2022.10.08.510936

Invited Talk CPP 30.4 Wed 10:15 TOE 317

Materials properties of bacterial biofilms. — •Cécile M. Bidan — Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Potsdam, Germany

As bio-sourced materials are raising interest for their sustainability, using bacteria to produce biofilms made of a protein and polysaccharide matrix has become a new strategy to make engineered living materials with various functionalities. Our group contributes to this emerging field by clarifying how bacteria adapt biofilm materials properties to the environment. For this, we culture E. coli producing curli amyloid and phosphoethanolamine-cellulose fibers on nutritive agar substrates with varying physico-chemical properties and study the growth, morphology and mechanical properties of the resulting biofilms. We demonstrated that changing the properties of the agar substrate with polyelectrolyte coatings or by varying the water content the bulk properties of the agar affects E. coli biofilm growth, morphology and mechanical properties. We also used E. coli producing only amyloid fibers and focus on the matrix structural and functional changes at the molecular scale. To assess the contribution of each matrix component to the macroscopic biofilm materials properties, we compared the characteristics of biofilms produced by a collection of E. coli mutants differing in the matrix they produce. The results indicate that E. coli biofilm matrix is a composite made of rigid and brittle curli amyloid fibers assembled within a mesh of soft and adhesive phosphoethanolamine-cellulose fibers. Finally, we explored how treating biofilms with ionic solutions can help tuning further their properties.

CPP 30.5 Wed 10:45 TOE 317

The migration and search behavior of immune cells — Reza Shaebani and •Franziska Lautenschläger — Saarland University, Saarbrücken

Immune cells have a variety of tasks in the body. For example, dendritic cells act as the *sentinels* searching for pathogens. For this search, the cells need to scan a certain area in an effective way. Here, we investigate how cells optimize the search of such area. We have shown before that all cell types show a correlation of migration speed and persistence [1]. We later found that cells which strongly correlate these two parameters are particularly good at searching objects [2]. Interestingly, we found that cells do not keep the memory of their speed as long as the memory of their persistence [3]. Now, we investigate how we can disturb this migration and search behavior, preferable by altering the cytoskeleton [4].

1.*Maiuri, P., et al., Actin flows mediate a universal coupling between cell speed and cell persistence. Cell, 2015. 161(2): p. 374-86. 2.*Shaebani, M.R., et al., Persistence-Speed Coupling Enhances the Search Efficiency of Migrating Immune Cells. Phys Rev Lett, 2020. 125(26): p. 268102. 3.*Shaebani, M.R., M. Piel, and F. Lautenschläger, Distinct Speed and Direction Memories of Migrating Cells Diversify Their Possible Search Strategies. arXiv. 4.*Shaebani, M.R., et al., Vimentin provides target search efficiency and mechanical resilience for dendritic cell migration. bioRxiv, 2020: p. 2020.12.18.423401.

CPP 30.6 Wed 11:00 TOE 317

Molecular motors from a 3D perspective: how do kinesins organize microtubules? — •Laura Meissner[1], Jonas Bosche[2], Ludger Santen[2], and Stefan Diez[1,3,4] — [1]B CUBE - Center for Molecular Bioengineering, TU Dresden, Dresden, Germany — [2]Center for Biophysics, Department of Physics, Saarland University, Saarbrücken, Germany — [3]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany — [4]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Kinesins are ubiquitous motor proteins that are essential for intracellular transport processes. In addition, several kinesins act within the mitotic spindle by sliding and crosslinking microtubules. Some of those kinesins not only move longitudinally on the microtubule filament but also display an axial component in their motion. So far, the effect of this axial motion on motility and force generation within the mitotic spindle has not been explored deeply. Using a 3D motility assay, we show that the antagonistic motor proteins kinesin-5 and kinesin-14 drive the rotation of microtubules around each other. We characterize their motility parameters, including velocity and pitch. Further, we determine the extension of the motors, which reveals the conformation of the motors in microtubule overlaps. To investigate the rotational force (torque) that the motors could produce during microtubule sliding, we developed a microtubule coiling assay. Here, both kinesin-5 and kinesin-14 bent and coiled microtubules, indicative of the generation of significant torque. We hypothesize that this behavior serves to organize spindle fibers and to provide robustness to the spindle.

15 min. break

CPP 30.7 Wed 11:30 TOE 317

3D stimulated Raman spectral imaging of water dynamics associated with pectin-glycocalyceal entanglement — •Moritz Floess[1], Tobias Steinle[1], Florian Werner[1], Yunshan Wang[1], Willi L. Wagner[2], Verena Steinle[2], Betty S. Liu[3], Yifan Zheng[3], Steven J. Mentzer[3], and Harald Giessen[1] — [1]4th Physics Institute, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Department of Diagnostic and Interventional Radiology, University Hospital of Heidelberg, Im Neuenheimer Feld 420, 69120 Heidelberg, Germany — [3]Laboratory of Adaptive and Regenerative Biology, Brigham & Women's Hospital, Harvard Medical School, Boston MA

Pectin, a heteropolysaccharide, is an ideal biomaterial for medical applications such as serosal wound healing and visceral tissue repair. It forms strong mechanical bonds with the underlying tissue. The extraordinary adhesive properties of pectin on organ surfaces are highly water-dependent and most likely result from a microstructural entanglement of pectin polysaccharide chains with the similarly textured glycocalyx, a glycoprotein coat, covering mammalian cell surfaces. We employ label-free 3D stimulated Raman scattering (SRS) microscopy to investigate the hydrophilicity of pectin hydrogel without the altering effects of sample fixation, dehydration, or tissue staining. In particular, we quantify the time scales, on which two different hydration mechanisms take place. Furthermore, the transition zone between pectin and porcine serosal tissue is imaged to obtain quantitative insights into the entanglement between pectin and mammalian glycocalyx.

CPP 30.8 Wed 11:45 TOE 317

Quantifying optomechanical properties of phase separated protein condensates — •Timon Beck[1], Lize van der Linden[2], Raimund Schlüssler[2], Kyoohyun Kim[1], Simon Alberti[2], and Jochen Guck[1] — [1]Max Planck Institute for the Science of Light, Erlangen, Germany — [2]Biotec TU Dresden, Dresden, Germany

The organization of intracellular material is a complex task and cells have different strategies for compartmentalization. One way is the formation of membraneless organelles that are involved, for example, in metabolic control and DNA repair. The underlying process of phase separation and percolation is tightly controlled by many parameters as temperature, ion and protein concentration, as well as crowding conditions. Changes in these parameters have an impact on the intermolecular interactions and accordingly tune optical and viscoelastic characteristics of the condensates. Despite the dynamic development of the research field in the last years, there is a lack of tools to quantitatively measure such physical properties. A combination of Brillouin microscopy with quantitative phase imaging, providing information about refractive index and density, gives access to a set of optical and mechanical quantities and in particular the longitudinal modulus. By varying temperature and ion conditions, we were able to tune intermolecular interactions within phase separated protein droplets and found that the introduced variations are reflected in the optomechanical properties of the condensates.

CPP 30.9 Wed 12:00 TOE 317

Confinement-induced fractionation and liquid-liquid phase separation of polymer mixtures — •Arash Nikoubashman[1] and Miho Yanagisawa[2] — [1]Institute of Physics, JGU Mainz, Germany — [2]Graduate School of Science, The University of Tokyo, Japan

The formation of (bio)molecular condensates via liquid-liquid phase separation in cells has received increasing attention, as these coacervates play important functional and regulatory roles within biological systems. However, the majority of studies focused on the behavior of pure systems in bulk solutions, thus neglecting confinement effects and the interplay between the numerous molecules present in cells. To advance our knowledge, we perform simulations of binary polymer mixtures in droplets, considering both monodisperse and polydisperse molecular weight distributions for the longer polymer species. We find that confinement induces a spatial separation of the polymers by length, with the shorter ones moving to the droplet surface. This partitioning causes a distinct increase of the local polymer concentration in the droplet center, which is more pronounced in polydisperse systems. Consequently, the systems exhibit liquid-liquid phase separation at average polymer concentrations where bulk systems are still in the one-phase regime.

CPP 30.10 Wed 12:15 TOE 317

Branching morphogenesis in the silica cell wall of diatoms — •Iaroslav Babenko[1,2,3], Benjamin M. Friedrich[1,2], and Nils Kröger[1,3] — [1]Cluster of Excellence Physics of Life, TU Dresden, 01062 Dresden, Germany. — [2]Center of Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany. — [3]Center for Molecular and Cellular Bioengineering, 01307 Dresden, Germany.

Diatoms live in a glass house: these common single-celled algae fascinated evolutionary biologists, chemical engineers and inspired artists for their ability to produce intricately nano- and micropatterned silica schells. The valve of the cell wall is formed in a planar intracellular compartment termed silica deposition vesicles (SDVs). The physical mechanism that guides the self-assembly of species-specific silica patterns is unknown. Here, we address this question by studying the formation of the silica rib patterns in the cell wall of the model diatom *Thalassiosira pseudonana* by combining theory and electron microscopy of nascent silica valves. We propose a minimal model of branching morphogenesis based on a non classical Turing reaction-diffusion system to quantitatively account for the time course of experimentally observed rib patterns. We introduce a novel mechanism of branching morphogenesis, which relies on a transition from soluble to insoluble silica phases inside the SDV and the concurrent release of an inhibitor that hinders this transition. Moreover, our minimal model is capable of producing a wide range of rib patterns, suggesting that this model may be applicable for describing branching morphogenesis in other diatom species and potentially, in other organisms.

CPP 30.11 Wed 12:30 TOE 317

Reimplementing the formation and dispersal of transcriptional clusters with synthetic DNA-nanomotifs and Langevin-dynamics simulations — •Aaron Gadzekpo[1], Xenia Tschurikow[1], Mai Tran[2], Rakesh Chatterjee[3,4], Vasily Zaburdaev[3,4], Kerstin Göpfrich[2], and Lennart Hilbert[1] — [1]Karlsruhe Institute of Technology — [2]Max Planck Institute for Medical Research — [3]Max Planck Zentrum für Physik und Medizin — [4]Friedrich-Alexander Universität Erlangen-Nürnberg

Spatial organisation of the genome is emerging as a crucial aspect of gene transcription. In pluripotent cells, self-interacting molecular factors, such as RNA polymerase II, form microphase-separated domains, which become increasingly dispersed due to amphiphilic effects of newly transcribed genes. To understand the principles that lead to this behaviour, we designed synthetic DNA-nanomotifs that form droplets due to self-interaction and allow for the addition of an amphiphilic tail of thymines. Time-lapse microscopy, titration experiments and analysis of the resulting distributions of droplet properties demonstrate that the synthetic system reproduces the dispersal of phase-separated domains found for increasing transcription levels. Simulations based on Langevin-dynamics equally reproduce this behaviour after tuning interaction strengths and number ratios. Our findings illustrate how model-guided design of DNA-based systems can elucidate the mechanisms that control spatio-temporal compartmentalisation in cells.

CPP 30.12 Wed 12:45 TOE 317

Partition complex structure can arise from sliding and bridging of ParB dimers — •Lara Connolley[1], Lucas Schnabel[2], Martin Thanbichler[2], and Sean Murray[1] — [1]Max Planck Institute for Terrestrial Microbiology, Marburg, Germany — [2]University of Marburg, Marburg, Germany

Chromosome segregation is vital for cell replication and in many bacteria is controlled by the ParABS system. A key part of this machinery is the association of ParB proteins to the parS-containing centromeric region to form the partition complex. Despite much work, the formation and structure of this nucleoprotein complex has remained unclear. It was recently discovered that CTP binding allows ParB dimers to entrap and slide along the DNA, as well as leading to more efficient condensation through ParB-mediated DNA bridging. Here, we use semi-flexible polymer simulations to show how these properties of sliding and bridging can explain partition complex formation. We find that transient ParB bridges can organise the DNA into either a globular state or into hairpins and helical structures, depending on the bridge lifetime. Upon coupling with stochastic sliding simulations to form a unified sliding and bridging model, we find that short-lived ParB bridges do not hinder ParB sliding and the model can reproduce both the ParB binding profile and the condensation of the nucleoprotein complex. Overall, our model clarifies the mechanism of partition complex formation and predicts its fine structure.

CPP 31: Focus Session: From Inter-individual Variability to Heterogeneous Group Dynamics and Disorder in Active Matter (joint session DY/BP/CPP)

The study of active particle dynamics has developed into a vibrant field of multidisciplinary research, including such diverse systems as bacterial colonies, cellular self-organization, synthetic colloids and microrobots as well as macroscopic systems like locusts, flocks of birds, schools of fish or pedestrians. Whereas many studies in the past focused either on the random transport of individual particles or on the interplay of temporal fluctuations (noise) and interactions (velocity alignment or attraction/repulsion), there is now an increasing interest in the question how structural disorder and inter-individual variability, i.e., different motility characteristics of individuals, shape the active particle dynamics and emergent pattern formation of groups. The presence of structural or quenched disorder raises furthermore the immediate question how to bridge data and models based on (short time) tracking data, given the simultaneous presence of temporal fluctuations. With this focus session, we aim at bringing researchers from statistical physics and biophysics together to discuss this interdisciplinary topic and exchange ideas on common challenges arising in different application areas.

Organized by Robert Großmann (Potsdam)

Time: Wednesday 9:30–13:00 Location: ZEU 160

Invited Talk CPP 31.1 Wed 9:30 ZEU 160

More is different: High-throughput 3D tracking reveals bacterial navigation strategies — •Katja Taute — Rowland Institute at Harvard, Harvard University, Cambridge, MA, USA — Department of Biology, Microbiology, LMU München, 82152 Martinsried, Germany

How microbes navigate environmental chemical gradients has implications that range from health to climate. The behavioral mechanisms underlying chemotaxis are unknown for most species because of a lack of techniques capable of bridging scales from individual navigation behavior to the resulting population-level performance. We present a multiscale 3D chemotaxis assay that combines high-throughput 3D bacterial tracking with microfluidically created chemical gradients. Large datasets of 3D trajectories yield the statistical power required to assess chemotactic performance at the population scale, while simultaneously resolving the underlying 3D navigation behavior for every individual. Applying this technique to the well-studied model bacterium Escherichia coli, we uncover dramatic, previously unknown heterogeneity in chemotactic performance. We investigate the underlying behavioral mechanisms and discuss potential implications at the population level.

Invited Talk CPP 31.2 Wed 10:00 ZEU 160

Variability and heterogeneity in natural swarms — •Gil Ariel — Bar Ilan University, Ramat Gan, Israel

Collective motion of large-scale natural swarms, such as moving animal groups or expanding bacterial colonies, have been described as self-organized phenomena. Thus, it is clear that the observed macroscopic, coarse-grained swarm dynamics depend on the properties of the individuals of which it is composed. In nature, individuals are never identical, and may differ in practically every parameter. Hence, intra-group variability and its effect on the ability to form coordinated motion is of interest, both from theoretical and a biological points of view. In this talk, I will review and examine some of the fundamental properties of heterogeneous collectives in nature, with an emphasis on two widely-used model organisms - swarming bacteria and locusts. Theoretical attempts to explain the observed phenomena will be discussed in view of laboratory experiments, highlighting their successes and failures. While heterogeneity typically discourages collectivity, there are several natural examples where it has an opposite effect.

CPP 31.3 Wed 10:30 ZEU 160

Effect of individual differences on the jamming transition in traffic flow — •Yi-Chieh Lai and Kuo-An Wu — Department of Physics, National Tsing Hua University, 30013 Hsinchu, Taiwan

The individual difference, particularly in drivers' distance perception, is introduced in the microscopic one-dimensional optimal velocity model to investigate its effect on the onset of the jamming instability seen in traffic systems. We show analytically and numerically that the individual difference helps to inhibit the traffic jam at high vehicle densities while it promotes jamming transition at low vehicle densities. In addition, the jamming mechanism is further investigated by tracking how the spatial disturbance travels through traffics. We find that the jamming instability is uniquely determined by the overall distribution of drivers' distance perception rather than the spatial ordering of vehicles. Finally, a generalized form of the optimal velocity function is considered to show the universality of the effect of the individual difference.

CPP 31.4 Wed 10:45 ZEU 160

Distinct impacts of polar and nematic self-propulsion on active unjamming — Varun Venkatesh[1], •Chandana Mondal[2], and Amin Doostmohammadi[1] — [1]Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, 2100 Copenhagen, Denmark — [2]UGC-DAE CSR, University Campus, Khandwa Road, Indore 452017, India

We explore, by MD simulations, the jamming-unjamming transition in a dense system of active semiflexible filaments. In particular, we characterize the distinct impact of polar vs nematic driving for different filament rigidities and at varying densities. Our results show that high densities of dynamic active filaments can be achieved by only changing the nature of the active force, nematic or polar. Interestingly, while polar driving is more effective at unjamming the system at high densities below confluency, we find that at even higher densities, nematic driving enhances unjamming compared to its polar counterpart. The effect of varying the rigidity of filaments is also significantly different in the two cases: While for nematic driving, lowering the bending rigidity unjams the system, we find an intriguing reentrant jamming-unjamming-jamming transition for polar driving as the filament rigidity is lowered. While the first transition (unjamming) is driven by softening due to reduced rigidity, the second transition (jamming) is a cooperative effect of ordering and coincides with the emergence of nematic order in the system. Together, through a generic model of self-propelled flexible filaments, our results demonstrate how tuning the nature of self-propulsion and flexibility can be employed by active materials to achieve high densities without getting jammed.

15 min. break

Invited Talk CPP 31.5 Wed 11:15 ZEU 160

Superstatistical Analysis and Modelling of Complex Dynamical Systems — •Claus Metzner[1,2], Christoph Mark[2], Ben Fabry[2], Patrick Krauss[1], Achim Schilling[1], Maximilian Traxdorf[3], and Holger Schulze[1] — [1]Neuroscience Lab, University Hospital Erlangen, Germany — [2]Biophysics Lab, Friedrich-Alexander Universität Erlangen-Nürnberg — [3]Department of Otorhinolaryngology, Head and Neck Surgery, Paracelsus Medical University, Nuremberg, Germany

On longer time scales, complex systems often pass through different dynamical attractors and thus produce 'anomalous' distributions and correlations when analyzed with conventional statistical tools. We argue that the most appropriate way of describing such systems is by hierarchical multilevel models, in which the lowest level is a relatively simple random walk model that can generate the observed time series on short time scales, but which depends on latent hyper-parameters that are themselves time-dependent and controlled by the higher levels of the model. First, our Bayesian method is introduced for the sequential inference of those gradual or abrupt parameter changes. We then review possible applications of the superstatistical framework in such diverse fields as biophysics, neuroscience, finance, or policy assessment. Finally, we discuss more recent extensions of the method for model selection and the use of machine learning models for estimating complex likelihood functions.

CPP 31.6 Wed 11:45 ZEU 160

How to infer parameter distributions in heterogeneous populations of active particles — •Jan Albrecht[1], Robert Grossmann[1], and Manfred Opper[2,3] — [1]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [2]TU Berlin, Fakultät IV-MAR 4-2, Marchstraße 23, 10587 Berlin, Germany — [3]Centre for Systems Modelling and Quantitative Biomedicine, University of Birmingham, B15 2TT, United Kingdom

Experiments with active particles, e.g., motile microorganisms like bacteria or amebae, provide information about their position at discrete points in time. However, most active particle models, like active Ornstein-Uhlenbeck particles for example, are commonly described by first order stochastic differential equations for the velocity or force. This leads to a second order model in position posing challenges for parameter inference, because there is no general way to obtain a closed form expression for the likelihood of the parameters in terms of those time-sampled trajectories. This would be needed to apply efficient Bayesian parameter estimation techniques. In this talk, we propose a filtering-like sequential method to address this problem. The likelihood is first expressed in terms of integrals over transition probabilities. Approximating the transition probability for small times makes these integrals analytically feasible, leading to a likelihood approximation that allows consistent parameter inference. Using a Bayesian approach, we furthermore show how to extend this framework to estimate the entire distribution of motility parameters in heterogeneous populations of particles efficiently.

CPP 31.7 Wed 12:00 ZEU 160

Derivation and analysis of a phase field crystal model for a mixture of active and passive particles* — •Michael te Vrugt[1,2], Max Philipp Holl[1], Aron Koch[1], Raphael Wittkowski[1,2,3], and Uwe Thiele[1,3,4] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Center for Soft Nanoscience — [3]Center for Nonlinear Science — [4]Center for Multiscale Theory and Computation

We discuss an active phase field crystal (PFC) model that describes a mixture of active and passive particles [1]. First, a microscopic derivation from dynamical density functional theory is presented that includes a systematic treatment of the relevant orientational degrees of freedom. Of particular interest is the construction of the nonlinear and coupling terms. This allows for interesting insights into the microscopic justification of phenomenological constructions used in PFC models, the approximations required for obtaining them, and possible generalizations. Second, the derived model is investigated using linear stability analysis and nonlinear methods. It is found that the model allows for a rich nonlinear behavior with states ranging from steady periodic and localized states to various time-periodic states. The latter include standing, traveling, and modulated waves corresponding to spatially periodic and localized traveling, wiggling, and alternating peak patterns and their combinations.

[1] MtV et al., Modelling Simul. Mater. Sci. Eng. 30, 084001 (2022)

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CPP 31.8 Wed 12:15 ZEU 160

Active Brownian Particles in a disordered motility environment — Gianni Jacucci[1], •Davide Breoni[2], Sandrine Heijnen[3], Hartmut Löwen[2], Giorgio Volpe[3], and Sylvain Gigan[1] — [1]Laboratoire Kastler-Brossel, Paris, France — [2]HHU Universität, Düsseldorf, Germany — [3]University College London, London, United Kingdom

The study of active matter, i.e. matter that consumes energy to perform actions, is fundamental to deepen the knowledge of living systems, as for example bacterial colonies or flocks of birds, and their collective behaviors. Complex environments, like the internal structure of a cell or a blood vessel, are of particular relevance in this field, as they provide a better description of the real-life settings typical of living matter.

In this work we study the effects of a disordered motility field on active Brownian particles, both in experiments and simulations. Experimentally, the motility field is generated by applying a speckle light field to thermophoretic Janus particles, in our case silica colloids half-coated with a carbon layer, suspended in a critical mixture of water and 2,6-lutidine. We focus on the differences between the effects of respectively a homogeneous and a disordered motility field on the dynamics of the particles.

CPP 31.9 Wed 12:30 ZEU 160

Characterization of spatial heterogeneities as influencing factors on the dynamics of confluent endothelial cell migration — •Anselm Hohlstamm, Andreas Deussen, Stephan Speier, and Peter Dieterich — Institut für Physiologie, TU Dresden

Confluent endothelial cells are in perpetual movement. Their collective dynamics arises from the interplay of self-propelled motility and various distance-related cell interactions. However, an understanding of collective cell dynamics is complicated by large spatial heterogeneities and local cluster formations. It is the aim of this work to quantify and characterize their influence on the dynamics of cell migration. We used human umbilical vein endothelial cells, which were stained with a fluorescent dye and observed for 48 hours via time-lapse microscopy. With automated image segmentation we could track several 10.000 cells. Cell densities and mean squared velocities showed a heterogeneous spatial distribution with an inverse relation to each other. Higher cell densities also affected the strength of the velocity autocorrelation, whereas correlation times remained mostly stable during experiments. However, cell division increased the mean squared velocity without changing temporal correlations. In parallel, the mean squared displacement characterized regions with short superdiffusive phases in an aging, highly non-stationary system. In addition, local dynamics are coupled by long range spatial correlations. In summary, the dynamics of an entire endothelial layer is influenced by interactions of small heterogenous regions. Next, we will use this approach to compare different endothelial cells.

CPP 31.10 Wed 12:45 ZEU 160

Exploiting the unknown - Smart nutrient collection surpassing the run and tumble strategy — •Mahdi Nasiri, Edwin Loran, and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

Throughout evolution, microorganisms have developed efficient strategies for locating nutrients and avoiding toxins in complex environments. Understanding their adaptive policies can provide new key insights for the development of smart artificial active particles. In this talk, we will present a novel method that uses deep reinforcement learning (DRL) to develop smart nutrient collection strategies for chemotactic active particles. Our method is complementary to our previous work which used DRL to explore optimal navigation [1] and is able to devise efficient survival strategies inside unknown and complex environments while only having access to local sensory data. We were also able to extract an interpretable model from the learned strategies which resemble striking similarities with the classical run and tumble motion.

[1] M. Nasiri, B. Liebchen, New J. Phys. 24, 073042 (2022).

CPP 32: 2D Materials IV (joint session HL/CPP)

Time: Wednesday 9:30–12:30 Location: POT 81

CPP 32.1 Wed 9:30 POT 81

Nonlinear optical characterization of atomically thin layers of the transition metal dichalcogenides WSe$_2$ and MoS$_2$ — •Henry Volker Hübschmann[1], Gerhard Berth[1], Ioannis Caltzidis[1], Katharina Burgholzer[2], Alberta Bonanni[2], and Klaus D. Jöns[1] — [1]Department of Physics, Paderborn University, 33098 Paderborn, Germany — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, 4040 Linz, Austria

In the field of quantum technologies functional 2D-structures based on transition metal dichalcogenides like WSe$_2$ and MoS$_2$ represent a novel material platform due to their specific optical and electronic properties. In contrast to semimetallic graphene they feature an electronic band gap and a strong spinorbit coupling. Applications of such layered 2D-materials in functional structures are to be found within photonics, spinorbitronics or nanoelectronics. In this work we present our fundamental nonlinear study on mechanically exfoliated atomically thin layers of the semiconductors WSe$_2$ and MoS$_2$. In this context, the second harmonic generation was determined for both van der Waals layered material systems as a function of the layer number. The respective nonlinear behavior was proven by a power-dependent characterization and supplemented by polarimetric analysis. Nonlinear imaging of the flakes was successfully performed by confocal SH-microscopy. In a further step the oxidation of MoS$_2$ layered systems was analyzed, here it was shown that for an even number of layers the oxidation leads to a break of their centrosymmetric structure, which is manifested in the clear presence of a relatively strong second harmonic signal.

CPP 32.2 Wed 9:45 POT 81

Single Photon Emitters in hBN via ultra-low energy helium ion implantation — •Prokhor Tkhor[1,2], Minh Bui[1,2], Renu Rani[1], Thorsten Brazda[1], and Beata E. Kardynał[1,2] — [1]Peter Grünberg Institut-9, Forschungszentrum Jülich, Jülich — [2]Department of Physics, RWTH Aachen, Aachen

Properties of heterostructures of transition metal dichalcogenides depend strongly on the moire lattice configuration and on the strength of coupling between the constituent monolayers. The first one can be controlled by the lattice constant of the constituent monolayers and their relative orientation, while the latter can be tuned by changing the spacing between them. In this contribution, we study a heterostructure of monolayers of WSe2/ hBN/ WSe2 with a moire potential periodicity of around 5 nm. The insertion of a monolayer of hBN between the two WSe2 monolayers results in a weak coupling between them. We discuss the results of the measurements of the dependence of the photoluminescence on the doping and electric field in this system. In this system the lowest intralayer excitonic states are optically spin-forbidden and at low electron concentration the effect of the moire potential on scattering of electrons and excitons dominates the optical signal masking the effect of correlations. Further, we discuss the observed non-monotonic charge shifts between the monolayers as a function of applied electric field.

CPP 32.3 Wed 10:00 POT 81

Thin hexagonal boron nitride in the deep-UV: The pursuit of single photon emitters and their properties — •Nils Bernhardt[1], Luka Choi[1], Felix Nippert[1], Angus Gentle[2], Milos Toth[2], and Markus R. Wagner[1,3] — [1]Technische Universität Berlin, Berlin, Germany — [2]University of Technology Sydney, Sydney, Australia — [3]Paul-Drude-Institut, Berlin, Germany

Interest in hexagonal boron nitride (hBN) continues to grow in optoelectronics with the discovery of an increasing number of quantum emitters in all spectral ranges. The wide band gap and chemical stability inherent to this material encourage hBN as a semiconductor substrate, while the possibility of reliably fabricating thin films entails unusual and unique properties. Consequently, room-temperature defect quantum emitters with reproducible emission properties from the UV to the near-IR can be engineered for applications such as quantum communication.

In this work, we investigate the recently observed luminescence of hBN at 4.1eV with a pulsed, frequency-tripled titanium-sapphire laser at 240nm. Experimental methods such as photoluminescence spectroscopy and time-resolved fluorescence spectroscopy are utilized alongside a Hanbury Brown and Twiss interferometer for correlation measurements in the deep UV as a means to identify single-photon emitters. Through this approach, we are able to establish a scientific basis for further investigation into the UV emission of hBN.

CPP 32.4 Wed 10:15 POT 81

Electrical control of excitonic complexes in MoSe$_2$ homobilayers — •Bárbara Rosa[1], Chirag Palekar[1], Alisson Cadore[2], Yuhui Yang[1], Aris Koula-Simos[1], Sefaattin Tongay[3], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [2]Brazilian Nanotechnology National Laboratory, Campinas, Brazil — [3]School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, USA

Effects of periodic Moiré potential in transition metal dichalcogenides (TMDs) bilayers are directly controlled by the twist angle between the monolayers. Novel features arising from intra- and interlayer excitons, such as their ultrafast formation and charger transfer, long population recombination lifetimes, and binding energy of dozens of meVs, turn TMD heterostructures into an attractive device for the study and manipulation of optical and transport properties via electrical fields. Moreover, such effects may appear even more pronounced at twisted homobilayers, since the absence of lattice mismatch promotes the appearance of larger Moiré superlattices. In this work, we explore the ability to control excitonic complexes in MoSe$_2$/MoSe$_2$ twisted bilayers (t-BLs) by performing gate-dependent microphotoluminescence (μPL) spectroscopy at room temperature. We observe the energy tunability of several meVs occurring at the emission of excitonic complexes derived from the t-BL region. In addition, other effects, such as the emergence of new excitonic features, are observed through μPL spectroscopy at cryogenic temperatures.

15 min. break

CPP 32.5 Wed 10:45 POT 81

Tailoring Coulomb interactions in WS$_2$-graphene heterostructures — •David Tebbe[1], Marc Schütte[1], Kenji Watanabe[2], Takashi Taniguchi[3], Christoph Stampfer[1], Bernd Beschoten[1], and Lutz Waldecker[1] — [1]2nd Institute of Physics A, RWTH Aachen University — [2]Research Center for Functional Materials, Japan — [3]International Center for Materials Nanoarchitectonics, Japan

The exciton binding energy and the quasiparticle bandgap in two dimensional semiconductors depend on their dielectric environment.

We investigate the screening of Coulomb interactions in heterostructures of WS$_2$ and graphene, separated through thin spacer layers of hexagonal boron nitride (hBN). By using hBN spacers from one to 16 atomic layers, we experimentally determine the tuning of the exciton binding energy and the quasiparticle bandgap as a function of the WS$_2$-to-graphene interlayer spacing.

This change in both energies is well described by a one over distance dependence, which is consistent with a screening arising from an image charge induced by the graphene layer.

Additionally, by doping the graphene with a graphitic back gate, we show that the ability of the graphene to screen Coulomb interactions in neighbouring layers is strongly modified. We determine the change in screening strength to be approximately 20% at room temperature, demonstrating that Coulomb-interactions in WS$_2$ can be modified insitu without changing the doping level of the material itself.

CPP 32.6 Wed 11:00 POT 81

Evidence for equilibrium exciton condensation in monolayer WTe2 — •Massimo Rontani — CNR-NANO, Modena, Italy

We present evidence [1] that the two-dimensional bulk of monolayer WTe2 contains electrons and holes bound by Coulomb attraction, excitons, that spontaneously form in thermal equilibrium. On cooling from room temperature to 100 K, the conductivity develops a V-shaped dependence on electrostatic doping, while the chemical potential develops a step at the neutral point. These features are much sharper than is possible in an independent-electron picture, but they can be accounted for if electrons and holes interact strongly and are paired in equilibrium. Our calculations from first principles show that the exciton binding energy is larger than 100 meV and the radius as small as 4 nm, explaining their formation at high temperature and doping levels.

Below 100 K, more strongly insulating behaviour is seen, suggesting that a charge-ordered state forms. The observed absence of charge density waves in this state is surprising within an excitonic insulator picture, but we show that it can be explained by the symmetries of the exciton wavefunction. Therefore, in addition to being a topological insulator, monolayer WTe2 exhibits strong correlations over a wide temperature range.

This work is done in collaboration with Elisa Molinari, Daniele Varsano, Samaneh Ataei, Maurizia Palummo, Bosong Sun, David Cobden. It is partially funded by MUR PRIN2017 No. 2017BZPKSZ EXC-INS and MaX EU Center of Excellence.

[1] B. Sun et al., Nature Physics 18, 94-99 (2022).

CPP 32.7 Wed 11:15 POT 81

Charge and exciton quenching at defect states in TMDC-graphene heterostructures — •Daniel Hernangómez-Pérez[1], Amir Kleiner[1], Andrea Donarini[2], and Sivan Refaely-Abramson[1] — [1]Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, 7610001 Rehovot, Israel — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

In recent years, studies of charge transfer and excitonic properties of van der Waals heterostructures have revealed a fertile research arena, spanning Coulomb blockade physics [1], ultrafast interlayer charge separation [2] or graphene-quenched photoluminescence [3]. We theoretically study charge transfer and excitonic properties in XS$_2$-graphene (X = W, Mo) heterobilayers with monoatomic chalcogen vacancies [4-5]. We discuss the impact of the subgap defect-based features in the microscopic dynamics, as well as the interplay between spatial symmetries and the spin degree of freedom through the spin-orbit interaction. Finally, we report the electronic and optical properties computed by many-body perturbation theory and show how defects and graphene alter the absorption properties of the TMDC due to a combination of folding, commensuration and impact of defect in-gap energy bands.

[1] N. Papadopoulos, *et al.* Phys. Rev. B 101, 165303 (2020). [2] S. Aeschlimann, *et al.* Science Advances 6 (20)(2020). [3] E. Lorchat, *et al.*, Nat. Nano. 15, 283 (2020). [4] D. Hernangómez-Pérez, A. Donarini, and S. Refaely-Abramson, arXiv:2209.14420. [5] D. Hernangómez-Pérez, A. Kleiner, and S. Refaely-Abramson (in preparation).

15 min. break

CPP 32.8 Wed 11:45 POT 81

The influence of anisotropy on excitons in magnetic semiconductors — •Marie-Christin Heissenbüttel, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Understanding the peculiar interrelation between crystal structure, magnetic properties and light-matter interaction in semiconducting two-dimensional-like magnets is of fundamental interest. From our ab-initio *GW*/Bethe-Salpeter equation calculations, we are able to examine electronic and excitonic properties on the same footing.

Because of its large crystal anisotropy combined with in-plane ferromagnetism, the van-der-Waals stacked CrSBr has recently come to the fore e.g. to study correlated phenomena. Due to the unique interplay of anisotropy, two-dimensional magnetism and optoelectronic properties resulting in a quantum confinement, we observe very flat dispersions, different effective masses and a quasi-1D behaviour of excitons within a monolayer of CrSBr [1]. Moreover, we find that the Rydberg series of two excitonic states is intricately modified by the different extension of the wavefunctions within momentum space.
[1] https://arxiv.org/abs/2205.13456

CPP 32.9 Wed 12:00 POT 81

From MoSe$_2$ to MoS$_2$ and everything in-between — •Jennifer Schmeink, Vladislav Musytschuk, Nicolas Hille, Erik Pollmann, Peter Kratzer, and Marika Schleberger — Universität Duisburg-Essen, Fakultät für Physik, Germany

Asymmetrical, or Janus transition metal dichalcogenide (TMDC) monolayers such as MoSSe are a current hot topic in the field of two-dimensional (2D) materials due to their unique properties. The most common approach of fabrication is to start off from one of the two base TMDCs' monolayer and selectively substitute the top-most layer of chalcogen atoms with another kind. However, if the substitution is partial, the resulting material resembles more an alloy than a Janus-type structure. These in-between materials show their own interesting features, as they allow for example a fluid optical bad-gap tuning from that of MoSe$_2$ at 1.54 eV over 1.70 eV for MoSSe up to 1.84 eV of MoS$_2$. In my talk I want to show off the varying optical and electronic properties of these $\text{MoS}_{2(1-x)}\text{Se}_{2x}$ $(0 \leq x \leq 1)$ structures with a special focus on the Janus-type MoSSe monolayer. This talk will explore the fascinating question of what lies in between.

CPP 32.10 Wed 12:15 POT 81

Optimized Irradiation Protocol for Quantum Sensors in Hexagonal Boron Nitride — •Paul Konrad[1], Andreas Gottscholl[1], Andreas Sperlich[1], Igor Aharonovich[2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, Julius-Maximilians-University of Würzburg, 97074 Würzburg — [2]School of Mathematics and Physical Sciences, University of Technology Sydney, Ultimo, NSW 2007, Australia

Colour centres in solid-state materials show great potential in quantum information technology and sensing applications. The lately discovered negatively charged boron vacancy (V_B^-) in hexagonal boron nitride (hBN)[1] has shown that the defect exhibits a spin-triplet ground state with spin-dependent photoluminescence. The system can be exploited in terms of its application as temperature, magnetic field, and pressure sensor [2,3] which extends the already known applications of e.g. NV-centers in diamond not only due to its 2D character but also by highly improved temperature sensing especially at low temperatures.

Here we present an irradiation protocol for creation of V_B^- by nitrogen ions, leading to optimized spin relaxation parameters and therefore improving quantum metrology limits. We also present tremendous improvement of ODMR contrast showing hyperfine interaction on flakes of down to 80nm thickness.

[1] Gottscholl et al., *Nat. Mat.*, **19**, 5, 540 (2020).

[2] Gottscholl et al., *Sci. Adv.*, **7** (14), eabf3630 (2021).

[3] Gottscholl et al., *Nat. Commun.*, **12**, 4480 (2021).

CPP 33: Perovskite and photovoltaics II (joint session HL/CPP)

Time: Wednesday 9:30–13:00 Location: POT 251

Invited Talk CPP 33.1 Wed 9:30 POT 251

Interfaces in perovskite optoelectronics: role of energy level alignment and interface chemistry — •Selina Olthof — Universität zu Köln, Institut für Physikalische Chemie

Optoelectronic devices, such as perovskite solar cells, are typically multi-layer stacks in which the absorber layer is sandwiched between metal oxide and/or organic transport layers in order to facilitate charge extraction or ensure charge selectivity. As the perovskite absorber layer has been extensively optimized in the past years, the awareness is rising that device efficiency and stability is limited by the interfaces present in the device. However, in perovskite-based devices, the role of this energy level alignment remains to be elusive and rather inconclusive studies can be found in literature, which I will briefly outline. More important for the device seems to be the perovskite composition at the interface which can be significantly influenced by chemical reactions taking place, in particular next to metal oxides. I will summarize our work on a variety of metal oxides in which we use photoelectron spectroscopy to analyze which components are responsible for the strong interface chemistry. We show that the reactivity strongly depends on the choice of perovskite and that different metal oxides show fundamentally different reaction/degradation pathways. Intriguingly, we are able to introduce surface treatments which change the surface defect density and thereby affect the degree of perovskite degradation significantly.

CPP 33.2 Wed 10:00 POT 251

Silver-nanoclusters and -vacancies influence the optical properties of Cs2AgBiCl6 nanocrystals — •Fei He[1], Yiou Wang[1], Quinten A. Akkerman[1], Markus Döblinger[2], Amrita Dey[1], and Jochen Feldmann[1] — [1]Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität, Königinstraße 10, 80539 Munich, Germany — [2]Department of Chemistry, Ludwig-Maximilians-Universität München, Butenandtstrasse 5-13 (E), 81377 München, Germany

Though being indirect semiconductors Cesium-Silver-Bismuth-Halides (so-called double perovskites) have attracted much attention as a nontoxic alternative to Lead Halide Perovskites. Novel applications for solar cells and X-ray detectors have already been developed.

Here, we report on the successful synthesis of spherical Cs2AgBiCl6 nanocrystals showing good stability and characteristic photoluminescent spectra. In transmission electron microscopy (TEM) images we observe Ag-clusters on the surface of the nanocrystals. It is known that silver ions are easily reduced into metallic Ag leading to silver vacancies in the double perovskite material and probably to Ag-clusters on the surface. We discuss how silver-nanoclusters and -vacancies influence the luminescent behavior of the double perovskite nanocrystals and explain possible microscopic origins.

CPP 33.3 Wed 10:15 POT 251

Accelerating research on solar cell materials with NOMAD — •Jose Marquez[1], Lauri Himanen[1], Markus Scheidgen[1], Claudia Draxl[1], Jens Hauch[2], Christoph Brabec[2], and Thomas Unold[3] — [1]Humboldt Universität zu Berlin — [2]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy — [3]Helmholtz-Zentrum Berlin

New solar cell technologies need decades to overcome the 20% power conversion efficiency threshold needed to make them commercially viable. With thousands of possible chemical compositions for new absorber layer materials and an unlimited number of possible device architectures, it becomes impossible to navigate this material space without the help of data science. To radically accelerate and democratize this development process, FAIR data management activities involving experimental solar cell data are needed. The NOMAD Laboratory (https://nomad-lab.eu) is a platform and open-source software driven by the NFDI consortium FAIRmat (https://fairmat-nfdi.eu) for making materials-science data FAIR. We show how the NOMAD infrastructure is evolving to support this task in the context of solar cells, demonstrated by an app for visualizing and searching rich and AI-ready experimental big solar cell data. NOMAD also provides an electronic lab notebook (ELN) which can be customized by research labs for AI-ready data/metadata entry, transfer, and processing in a FAIR-database context.

CPP 33.4 Wed 10:30 POT 251

Interdiffusion of Cu(In,Ga)Se2 and Ag(In,Ga)Se2 investigated by In-Situ X-Ray Diffraction — •Julia Horstmann[1], Roland Mainz[2], Karsten Albe[3], Heiko Kempa[1], Torsten Hölscher[1], and Roland Scheer[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Helmholtz-Zentrum Berlin, Germany — [3]Technische Universität Darmstadt, Germany

The partial substitution of Ag with Cu in the chalcopyrite-based absorber of thin film solar cells is a promising approach towards higher power conversion efficiencies. The resulting (Ag,Cu)(In,Ga)Se2 (ACIGSe) alloy achieves a bandgap widening up to 0.2 eV, increased grain growth and a lower melting temperature. The latter might reduce structural defects and therefore recombination losses in the absorber. This is favorable especially for wide-bandgap solar cells, used as top subcells in tandem devices, whose device performance is mainly limited by deep defects. To gain a better understanding of the diffusion on the (I) sublattice, we experimentally explored the interdiffusion of Cu(In,Ga)Se2 and Ag(In,Ga)Se2 layers by in-situ X-ray diffraction (IS-XRD) and glow discharge optical emission spectroscopy. Besides the positive aspects of Ag-alloying, thermodynamic simulations have shown a miscibility gap for temperatures between 100°C and 400°C. It is theoretically proposed, that ACIGSe with a high Ga content and with a [Ag]/([Ag]+[Cu]) ratio between 0.25 and 0.75 decomposes into Ag-rich and Ag-poor phases. We have studied the phase stability of Ga-free and Ga-rich samples using IS-XRD during post-annealing processes.

CPP 33.5 Wed 10:45 POT 251

NiO in perovskite solar cells: a peculiar interplay of degradation, passivation and device performance — •John Mohanraj[1], Bipasa Samanta[2], Maytal Caspary Torokar[2], and Selina Olthof[1] — [1]University of Cologne, 50939 Cologne, Germany — [2]Technion - IIT, Haifa, 3200003 Israel

The degradative interactions at the NiO/perovskite interface are notorious in the perovskite community as they lead to significant Voc and stability losses in p-i-n type perovskite solar cells (PSCs). So far, various Lewis bases have been introduced at this interface to passivate the metal oxide surface defects. Despite this process being successful in minimizing Voc and stability losses in PSCs, in-depth understanding of surface passivation and consequent suppression of the chemical processes at the NiO/perovskite interface are still elusive. This calls for a comprehensive surface investigation. To address these issues, we investigated solution processed NiO surfaces, their treatment with a series of passivating compounds, and the interface towards MAPbI3 in order to systematically probe the interface stability. Our methods include X-ray and UV photoelectron spectroscopy (XPS/UPS), XRD, SEM and UV-Vis absorption techniques. In parallel, first principle DFT calculations on differently treated NiO/MAPbI3 interfaces were carried out. These complementary investigations reveal changes in surface composition of the treated NiO and help us to suggest possible mechanisms for the degradative interactions. Finally, PSCs were fabricated using the stabilized NiO interfaces, and the impact on photovoltaic characteristics and device stability have been investigated.

30 min. break

CPP 33.6 Wed 11:30 POT 251

Resonant coupling of spin-flip excitations with phonons in BiFeO3 — •Aseem Rajan Kshirsagar and Sven Reichardt — Department of Physics and Material Science, University of Luxembourg, Luxembourg

BiFeO3 is a technologically relevant multiferroic perovskite. While a vast literature exists on its electronic, optical, and multiferroic properties, some of its optically active electronic excitations remain to be understood or have been interpreted in ambiguous ways. This applies in particular to features below the absorption onset that feature prominently in resonant Raman scattering [1]. Here we present a detailed study of the electronic structure and resonant Raman spectrum of BiFeO3 from first principles. Using many-body perturbation theory on top of density functional theory, we first analyze and characterize its optical absorption spectrum in terms of excitons and atomic orbitals, focusing in particular on spin-flip excitations that are strongly localized. We then use the state-of-the-art method for the ab initio calculation of resonant Raman intensities [2,3] to analyze the resonant coupling of these finite-spin excitations with phonons. Our results show that these only weakly optically active excitations still leave a clear imprint on the resonant Raman spectrum, making the latter an even more powerful tool to probe "darker" electronic excitations.

[1] M. C. Weber, et al. Phys. Rev. B, 93, 125204 (2016).
[2] S. Reichardt and L. Wirtz, Phys. Rev. B, 99, 174312 (2019).
[3] S. Reichardt and L. Wirtz, Sci. Adv., 6, eabb5915 (2020).

CPP 33.7 Wed 11:45 POT 251

Coherent Phonons in Halide Perovskite Nanocrystals — •Julian Georg Mann[1], Fei He[1], Quinten Akkerman[1], Tushar Debnath[2], and Jochen Feldmann[1] — [1]Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany — [2]Centre for Nanotechnology, Indian Institute of Technology Guwahati, Guwahati-781039

Halide perovskite nanocrystals are gaining increasing attention in contemporary research due to their promising performance in both light-emitting and solar technologies. We recently showed that photoexcitation of halide-perovskite nanocrystals with ultrashort laser pulses produces coherent phonons (Nat. Comm. 12, 2629 (2021)). We report femtosecond pump-probe spectroscopy studies on the formation and dynamics of coherent phonons in formamidine lead-halide (FAPbX$_3$) nanocrystals in terms of higher harmonic vibrational modes. In addition, we investigate the dynamics of vibrational wave packets in spherical Cs$_2$AgBiBr$_6$ double perovskite nanocrystals. Here, we observe that optically launched vibrational wave-packets alter spectral positions of excitonic resonances or oscillator strength of particular electronic transitions. Our results show that electron-phonon couplings (polaronic effects) need to be considered to fully understand the optoelectronic properties of halide-perovskite semiconductors.

CPP 33.8 Wed 12:00 POT 251

Phonon-driven Intra-exciton Rabi Oscillations in Halide Perovskites — •Katrin Winte[1], Xuan Trung Nguyen[1], Daniel Timmer[1], Davide Ceratti[2], Caterina Cocchi[1], Michael Lorke[3], Frank Jahnke[3], David Cahen[2], Christoph Lienau[1], and Antonietta De Sio[1] — [1]University of Oldenburg, Germany — [2]Weizmann Institute of Science, Israel — [3]University of Bremen, Germany

There is increasing consensus that in halide perovskites (HaPs) the interaction of electronic excitations with the phonon modes of their flexible polar lattice is crucial for the unique optoelectronic and transport properties of these materials. Here we show that coherent low frequency phonon of the lead-halide lattice induce Rabi oscillations between 1s and 2p excitons in CsPbBr$_3$ crystals. Ultrafast two-dimensional electronic spectroscopy reveals an excitonic peak structure oscillating with a 100-fs period up to 2 ps at 20 K. This frequency does not match any phonon modes of the crystals. Only after 2 ps, slow coherent phonon oscillations dominate the dynamics. We rationalize these findings as off-resonant intra-exciton Rabi oscillations induced by the Pb-Br phonon fields of the HaP crystals. We show that the slow motion of Pb-Br sublattice induces electric fields at THz frequencies that are sufficiently strong to drive off-resonant population oscillations between 1s and 2s excitons. Model simulation of the nonlinear optical response support this interpretation. This goes beyond prevailing models for the electron-phonon coupling in HaPs. It suggests that the coupling of characteristic low frequency phonon to intra-excitonic transitions may be the key to control their anharmonic response.

CPP 33.9 Wed 12:15 POT 251

Determining (almost) all optoelectronic properties of halide perovskites by transient photoluminescence — •Hannes Hempel[1], Martin Stolterfoht[2], Fangyuan Ye[2], and Thomas Unold[1] — [1]Helmholtz Zentrum Berlin, Germany — [2]Institute of Physics and Astronomy, University of Potsdam, Germany

Time-resolved photo luminescence (trPL) is probably the most common technique to quantify lifetimes of photogenerated charge carriers in semiconductors. However, the usual fitting of exponential decays to estimate lifetimes is a rather crude phenomenological approach since it ignores quenching processes that are not connected to carrier recombination and disregards the absolute amplitude of the luminescence. Here, we present an analysis of injection-dependent absolute trPL transients of bare triple-cation lead halide perovskite thin films. The presented analysis reveals a doping concentration of 3x1013cm-3 and a charge carrier mobility of 0.8 cm2/Vs, which are confirmed by Hall measurements. Further, we determine the injection-dependence of external radiative lifetimes, of the external radiative coefficient, and of the effective charge carrier lifetime. Based on the properties, an implied current-voltage curve is constructed that reveals the potential performance of the material in solar cell. Our trPL-based approach agrees well with the results of injection-dependent photoluminescence quantum yield measurements. However, it is superior in attributing losses, e.g. in the radiative ideality factor or the implied open circuit voltage, to the internal optoelectronic properties and thereby indicates the path to overcome these losses.

CPP 33.10 Wed 12:30 POT 251

Characterization of optoelectronic properties of CsSnI3 perovskite thin film as a function of chemical composition. — •Fatima Akhundova, Hannes Hempel, Marin Rusu, Elif Hüsam, Marcus Bär, and Thomas Unold — Helmholtz-Zentrum Berlin

The performance of lead-based halide perovskites as a next generation solar cell rises every year, however toxicity of Pb is a major obstacle for commercialization. Tin is the immediate substitute for Pb in perovskite crystal structure as both metals possess the same electronic configuration. However, Sn-perovskite solar cells have significantly lower efficiencies which is partially caused by poor stability of Sn(II). We report a systematic study of structural and optoelectronic properties of co-evaporated CsSnI3 thin films with regard to lateral compositional gradient. Elemental compositions are confirmed by X-ray fluorescence and X-ray photoelectron spectroscopy techniques. Grazing-incidence X-ray diffraction reveals orthorhombic gamma phase with different preferred orientation for the excess Sn and Cs content. Moreover, Cs-rich regions shows better phase stability than the Sn-rich parts which undergo a phase transition to non-perovskite phase. The optical band gap, work function, and ionization energy are measured as a function of the Cs:Sn ratio to characterize the band diagram. The photoluminescence quantum yield, the charge carrier lifetime and mobility present these properties are rather robust against changes in composition. Our work emphasizes the impact of chemical composition on optoelectronic properties of Sn-based perovskites and demonstrates agile strategy for compositional engineering in materials research.

CPP 33.11 Wed 12:45 POT 251

FAIR Cesium Lead Halide Perovskites Data by High-Throughput Investigation of Co-Evaporated Combinatorial Libraries — •Hampus Näsström[1], Pascal Beblo[2], Fatima Akhundova[2], Oleksandra Shargaieva[2], Jose A. Marquez[1], Hannes Hempel[2], Andrea Albino[1], Sebastian Brückner[1], Claudia Draxl[1], Eva Unger[2], and Thomas Unold[2] — [1]Humboldt-Universität zu Berlin — [2]Helmholtz-Zentrum Berlin

Artificial intelligence presents new possibilities in experimental materials research but typically require large well-characterized datasets. High-throughput technologies, including combinatorial synthesis, provide one method for obtaining such datasets. In this work, we show how such a dataset can be created through combinatorial co-evaporation and high-throughput characterization of Cs$_y$Pb$_{1-y}$(Br$_x$I$_{1-x}$)$_{2-y}$ perovskites. The evaporated films were investigated with a multitude of contact-less characterization methods such as hyperspectral photoluminescence imaging, time-resolved photoluminescence mapping, and grazing-incidence wide-angle X-ray scattering mapping. The results were combined to estimate the potential of the material in terms of the photovoltaic power conversion efficiency as a function of the Cs to Pb and Br to I ratio. Finally, a generalized data schema for combinatorial thin films was developed, and the data of the 3456 individual samples was disseminated in a Findable, Accessible, Interoperable and Reusable (FAIR) way within the Novel Materials Discovery (NOMAD) laboratory (nomad-lab.eu) that is operated by the NFDI consortium FAIRmat (fairmat-nfdi.eu).

CPP 34: Wetting, Droplets and Microfluidics I (joint session DY/CPP)

Time: Wednesday 10:00–13:00 Location: ZEU 147

CPP 34.1 Wed 10:00 ZEU 147

Crises and chaotic scattering in hydrodynamic pilot-wave experiments — George Choueiri[1,2], Balachandra Suri[1,3], Jack Merrin[1], Maksym Serbyn[1], Björn Hof[1], and •Nazmi Burak Budanur[1,4] — [1]Institute of Science and Technology Austria, 3400 Klosterneuburg, Austria — [2]MIME Department, University of Toledo, Toledo, Ohio 43606, USA — [3]Department of Mechanical Engineering, Indian Institute of Science, Bengaluru 560012, India — [4]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Theoretical foundations of chaos have been predominantly laid out for finite-dimensional dynamical systems, such as the three-body problem in classical mechanics and the Lorenz model in dissipative systems. In contrast, many real-world chaotic phenomena, e.g., weather, arise in systems with many (formally infinite) degrees of freedom, which limits direct quantitative analysis of such systems using chaos theory. In the present work, we demonstrate that the hydrodynamic pilot-wave systems offer a bridge between low- and high-dimensional chaotic phenomena by allowing for a systematic study of how the former connects to the latter. Specifically, we present experimental results, which show the formation of low-dimensional chaotic attractors upon destabilization of regular dynamics and a final transition to high-dimensional chaos via the merging of distinct chaotic regions through a crisis bifurcation. Moreover, we show that the post-crisis dynamics of the system can be rationalized as consecutive scatterings from the nonattracting chaotic sets with lifetimes following exponential distributions.

CPP 34.2 Wed 10:15 ZEU 147

Chemically Active Wetting — •Susanne Liese[1], Xueping Zhao[2], Frank Jülicher[3], and Christoph Weber[1] — [1]Universität Augsburg, Augsburg, Germany — [2]Xiamen University, Xiamen, China — [3]MPI/PKS, Dresden, Germany

In living cells, wetting of condensed phases on membrane surfaces provides a mechanism for positioning biomolecules. Biomolecules are also able to bind to such membrane surfaces. In living cells, this binding is often chemically active as it is kept out of equilibrium by the supply of energy and matter. Here, we investigate how active binding on membranes affects the wetting of condensates. To this end, we derive the non-equilibrium thermodynamic theory of active wetting. We find that active binding significantly alters the wetting behavior leading to non-equilibrium steady states with condensate shapes reminiscent of a fried egg or a mushroom. We further show that such condensate shapes are determined by the strength of active binding in the dense and dilute phases, respectively. Strikingly, such condensate shapes can be explained by an electrostatic analogy where binding sinks and sources correspond to electrostatic dipoles along the triple line. Through this analogy, we can understand how fluxes at the triple line control the three-dimensional shape of condensates.

CPP 34.3 Wed 10:30 ZEU 147

Stimuli-responsive high aspect ratio surfaces for wetting studies — •Gissela Constante[1], Indra Apsite[1], Paul Auerbach[2], Sebastian Aland[2], Dennis Schönfeld[3], Thorsten Pretsch[3], Pavel Milkin[1], and Leonid Ionov[1,4] — [1]Uni Bayreuth, Bayreuth, Germany — [2]HTW Dresden, Dresden, Germany — [3]Fraunhofer IAP, Postdam, Germany — [4]Bavarian Polymer Institute, Bayreuth, Germany

The fabrication of switchable surfaces has been of interest in different fields such as biotechnology, industry, robotics, and others. The fabrication of these shape-changing bioinspired surfaces is a challenge due to the limited availability of materials and methods. In this research, an exceptional high aspect ratio lamellar surface topography was fabricated by melt-electrowriting of microfibers of a shape-memory thermo-responsive polyurethane. Two different types of stimuli: temperature and light exposition were applied to modify the mechanical properties and by it the deformation and recovery of the original surface. Wetting studies showed that the deformation of the high aspect ratio lamellar surface can be tunned not only manually, but as well by a liquid droplet. This behavior is controlled by variation of temperature conducted by direct heating/cooling or by exposure to light when the lamellae were stained with black ink. The liquid in combination with thermo-responsive topography presents a new type of wetting behavior. This feature opens the possibility to apply such topographies for the design of smart elements for microfluidic devices, for example, smart valves.

CPP 34.4 Wed 10:45 ZEU 147

A Study about Shock-Induced Spallation in Mono- and Nanocrystalline High-Entropy Alloys — •Daniel Thürmer[1], Nina Merkert née Gunkelmann[1], Shiteng Zhao[2], Orlando Deluigi[3], Camelia Stan[4], Iyad Alhafez[5], Herbert Urbassek[5], Marc Meyers[6], and Eduardo Bringa[3,7] — [1]Institute of Applied Mechanics, Clausthal University of Applied Technology, Arnold-Sommerfeld-Stra*e, D-38678 Clausthal-Zellerfeld, Germany — [2]School of Material Science and Engineering, Beihang University, 37 Xueyuan Rd, Haidian District, Beijing, China, 100191 — [3]CONICET and Faculty of Engineering, University of Mendoza, Mendoza, 5500, Argentina — [4]Advanced Light Source Facility, Lawrence Berkeley National Laboratory, One Cyclotron Road, Berkeley, CA 94720, United States — [5]Physics Department and Research Center OPTIMAS, University Kaiserslautern, Erwin-Schr*odinger-Stra*e, D-67663 Kaiserslautern, Germany — [6]Mechanical and Aerospace Department, Univ. of California San Diego, La Jolla, CA 92093, United States — [7]Centro de Nanotecnología Aplicada, Universidad Mayor, Santiago, Chile

High-entropy alloys are highly attractive for future applications in the technical field thanks to their incredible potential regarding mechanical properties. Although they are increasingly sparking interest for future usage, their general understanding is not yet complete. To further understand high-entropy alloys and their capabilites, we studied the influence of shock-induced spallation on mono- and nanocrystalline high-entropy alloys with varying grain sizes.

CPP 34.5 Wed 11:00 ZEU 147

Instability of Active Fluid Interfaces in Microfluidics — •Kuntal Patel and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

In recent years, microfluidic lab-on-a-chip devices have emerged as efficient miniaturized flow control platforms. Specifically, the advent of nonlinear microfluidics has opened a new avenue for chemical and biomedical applications such as droplet formation and cell sorting. In this work, we integrate ideas from active matter into a microfluidic setting and try to understand the mechanism and practical relevance of resulting microfluidic flows.

The present setup consists of two vertically stacked fluid layers with identical densities but different viscosities, sandwiched between the walls of a microfluidic channel. The interface separating both fluids is initialized with uniformly distributed active particles, which induce force dipoles that generate flows in the adjacent fluids.

Our hybrid lattice-Boltzmann finite-difference simulations reveal that when we perturb the fluid interface covered with extensile force dipoles $\overset{\uparrow}{\downarrow}$, it eventually returns to its flat state irrespective of the strength of interfacial tension. In contrast, contractile force dipoles $\overset{\downarrow}{\uparrow}$ lead to activity-driven interfacial instability. However, such instability emerges only above a critical value of the activity, which is proportional to the interfacial tension. We further examine the mechanism of instability and quantify the effect of viscosity contrast and perturbation wavelength. Lastly, we demonstrate the systematic formation of droplets using the present interfacial instability.

CPP 34.6 Wed 11:15 ZEU 147

Optically controlled micro-transport with reduced heating impact — •Antonio Minopoli, Elena Erben, Susan Wagner, and Moritz Kreysing — Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Recently it was demonstrated that thermoviscous flows can be used to move the cytoplasm of cells and developing embryos. These laser-induced intracellular flows (aka FLUCS), reach velocities comparable with those occurring during early stages of embryogenesis. As a side effect, the laser scanning may also cause temperature gradients across the sample (1-3 Kelvins) that could give rise to out-of-equilibrium phenomena. Here, we demonstrate that exploiting symmetry relations during the laser scan, we disentangle heating and flows. Specifically, since the flow speeds depend on the repetition frequency rather than on the beam velocity, it is possible to accelerate the scanning of the primary scan pattern, effectively compressing the scan signal to occupy only a fraction of the original period, and allowing to complement the flow stimuli by flow-invariant heat stimuli. We introduce strategies to complement even complex primary scan patterns by secondary heating stimuli thereby yielding a near isothermal temperature distribution and still generating significant net flows. As we experimentally show, the resulting temperature distributions are near homogenous across the sample (standard deviations 5-10 times lower than those measured with standard FLUCS) and can therefore be better compensated for by ambient cooling. In the next future, ISO-FLUCS may become the new standard for optofluidic manipulations within biological systems.

15 min. break

CPP 34.7 Wed 11:45 ZEU 147

3D passive non-mechanical microfluidic valves fabricated using grayscale lithography — •Sebastian Bohm[1,3], Hai Binh Phi[2,3], Erich Runge[1], Lars Dittrich[3], and Steffen Strehle[2] — [1]TU Ilmenau, FG Theoretische Physik I — [2]TU Ilmenau, FG Mikrosystemtechnik — [3]5microns GmbH, 98693 Ilmenau

Passive non-mechanical valves represent a promising method for rectifying flows in micro- or nanofluidic systems [1]. They are very robust due to the absence of mechanical parts, easy to fabricate, and allow the implementation of efficient microfluidic systems such as micropumps [2,3]. However, with existing methods, the fabrication of fully three dimensional (3D) structured geometries is very hard to achieve. Here, a new and easy to implement method for the fabrication of three-dimensional valves is presented: Grayscale lithography followed by a proportional transfer with reactive ion etching is utilized to create 3D diffuser valves in silicon and glass substrates. We show that higher diodicities were achieved with 3D diffuser valves compared to conventional diffuser valves. These experimental findings correspond fit very well to the predictions of our numerical simulations. In combination with highly efficient optimization methods for two-dimensional Tesla valves, the fabrication of even more efficient 3D Tesla valves is hence now within reach.

[1] Bohm, S. et al.; npg Microsystems & Nanoengineering (8), 97 (2022)
[2] Bohm, S. et al.; COMSOL Conference 2020 Europe, 14-15. Oct. 2020 online
[3] Hoffmann, M. et al.; German patent DE112011104467 (2017)

CPP 34.8 Wed 12:00 ZEU 147

Coalescence of nematic droplets in quasi 2D liquid crystal films — •Christoph Klopp and Ralf Stannarius — Otto von Guericke University, Institute of Physics

Coalescence of droplets is ubiquitous in nature and modern technology. Various experimental and theoretical studies explored droplet dynamics in three dimensions (3D) and on two-dimensional (2D) solid or liquid substrates, e.g. [1-4]. Here, we demonstrate coalescence experiments of isotropic and nematic droplets in quasi-2D liquids, viz. overheated smectic A freely suspended films. We investigated their dynamics experimentally and measured the shape deformation during the entire merging process using high-speed imaging and interferometry. This system is a unique example where the lubrication approximation can be directly applied, and the smectic membrane plays the role of a precursor film. Our studies reveal the scaling laws of the coalescence time depending on the droplet size and the material parameters. We also compared the dynamics of isotropic and nematic droplets and additionally analyzed the results based on an existing model for liquid lens coalescence on liquid and solid surfaces [4].

This study was supported by DLR with project 50WM2054 and by DFG with project STA 425/40.

References:

[1] J. D. Paulsen et al., Nat. Commun., 5, 3182 (2014) [2] D. G. A. L. Aarts et al., Phys. Rev. Lett., 95, 164503 (2005). [3] M. A. Hack et al., Phys. Rev. Lett. 124, 194502 [4] N. S. Shuravin et al., Phys. Rev. E, 99, 062702 (2019) [5] C. Klopp et al., Langmuir, 36, 10615 (2020)

CPP 34.9 Wed 12:15 ZEU 147

effect of deposition method on the static contact angle of nanodroplets measured by AFM — •mohammadali hormozi and regine von klitzing — soft matter at interface, tu darmstadt, darmstadt, Germany

The wetting properties of substrates are often described by the static contact angle of a particular liquid. The contact angle depends on many parameters like substrate chemistry, liquid properties, and environment condition. In this study, we show that the method of depositing the liquid phase on the solid phase can play an important role for the static contact angle. For this purpose, microscale droplets of non-volatile liquids including Polyethylene Glycol (PEG200) and Squalane are deposited on the silanized substrate using four different methods. These methods are either based on nucleation (condensation and solvent exchange) or printing (inkjet and microcontact printing) of droplets. The contact angle of the microdroplets is scanned with an AFM and allows detailed analysis of the three phase contact line on a nm scale. The final static contact angle of the microdroplets is compared with the macroscopic contact angle determined by optical methods. Droplets formed via nucleation show smaller contact angle than printed ones. The latter ones were closer to the macroscopic contact angle. We will discuss this phenomenon.

CPP 34.10 Wed 12:30 ZEU 147

Fingering contact propagation between a droplet and a thin liquid film — •Kirsten Harth — Fachbereich Technik, TH Brandenburg — MRTM und MARS, Otto von Guericke Universität Magdeburg

When impacting droplets approach a hard plane substrate slowly, so that the Weber number is below approximately 5, a contact-less rebound will occur due to the entrainment of ambient gas. On slightly deformable and smooth spin-coated liquid films upon a rigid solid, this effect is more robust and may occur until slightly higher Weber numbers. Deformation of the thin film is usually ignored while it is proven to be present. The deformation amplitude depends on the impact dynamics as well as the thickness and viscosity of the surficial oil layer. At slightly higher impact velocities, i.e. slightly higher Weber numbers, delayed contact formation between the film liquid and the droplet occurs. Depending on the layer properties, interestingly, the contact line may be unstable displaying a fingering texture. Instability occurs independently of whether the drop and film liquid differ or not. We present and analyze this phenomenon.

CPP 34.11 Wed 12:45 ZEU 147

Universality in One-Dimensional Breath Figures — •Daniel Dernbach, Adrian Häussler-Möhring, M Muhammad, and Jürgen Vollmer — Institut für Theoretische Physik, Universität Leipzig, Brüderstr. 16, D-04103 Leipzig, Germany

Patterns of droplets which condense upon substrates reveal self-similar features. They are described by a scaling theory with a non-trivial exponent that has been related to the fractal dimension of the scaling of the free area (“porosity”) in between droplets. There is no agreement if this exponent is universal or affected by the dynamics. Here, we present numerical data that address the dependence of the asymptotic scaling of the porosity for hyper-spherical droplets growing on one-dimensional substrates. We vary the droplet dimension and interactions. For a given dimension the exponent is universal up to a critical range of interaction. For longer-ranged interactions the scaling depends on the dynamics.

CPP 35: Poster Session II

Topics: Biopolymers, Biomaterials and Bioinspired Functional Materials (1-5); Complex Fluids and Colloids, Micelles and Vesicles (6-13); Composites and Functional Polymer Hybrids (14-23); Crystallization, Nucleation and Self-Assembly (24-32); Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods (33-41); Hydrogels and Microgels (42-44); Modeling and Simulation of Soft Matter (45-50); Nanostructures, Nanostructuring and Nanosized Soft Matter (51-52); Polymer and Molecular Dynamics, Friction and Rheology (53-57); Responsive and Adaptive Systems (58-61); Wetting, Fluidics and Liquids at Interfaces and Surfaces (62-66).

Time: Wednesday 11:00–13:00 Location: P1

CPP 35.1 Wed 11:00 P1

Stability of biobased coatings on textiles — •Luciana Pluntke[1,2], Constantin Harder[1,3], Shouzheng Chen[1,4], Iuliana Ribca[5], Nadja Kölpin[1], Markus Oberthür[2], Peter Müller-Buschbaum[3], Mats Johansson[5], and Stephan V. Roth[1,5] — [1]DESY, 22607 Hamburg, Germany — [2]HAW, 20999 Hamburg, Germany — [3]TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, 85748 Garching, Germany — [4]University Hamburg, 20146 Hamburg, Germany — [5]KTH Royal Institute of Technology, 10044 Stockholm, Sweden

Functionalizing textiles by spray-coating is in wide-spread use. Here, we focus on functional multi-layer protective coatings on light woven textile materials. The functionalization is achieved by spray-coating with bio-based materials.

We investigate the mechanical stability of these novel coatings and changes in the coating under external stress and standard abrasion conditions. Our aim is to determine the degree of stress that the coating can withstand under different types of mechanical stress until it loses it functionality. The results are important for implementing sustainable materials in textile industry.

CPP 35.2 Wed 11:00 P1

In situ GISAXS printing of biotemplated titania nanostructures — •Linus F. Huber[1], Manuel E. Scheel[1], Stephan V. Roth[3], and Peter Müller-Buschbaum[1,2] — [1]Technical University of Munich,TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, James-Franck-Str. 1, 85748 Garching, Germany — [2]MLZ,TUM, 85748 Garching — [3]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Hamburg, Germany

Biotemplating is an effective method of nanostructuring hybrid inorganic-organic materials. This approach allows the tuning of material properties like porosity or domain sizes. Therefore, parameters like the electronic conductivity can be adjusted for different applications. In this work, differently structured Titania thin films are investigated for application in thermoelectric generators. Beta-lactoglobulin is a bovine whey protein that is used as a template during sol-gel synthesis. The Seebeck effect allows the conversion of waste heat into electrical energy. State of the art thermoelectric materials are rare, toxic and expensive. Biotemplated titania could provide a non-toxic and abundant alternative. To investigate the different titania morphologies, in situ GISAXS, GIWAXS and SEM are used. In situ GISAXS printing enables a time resolved investigation of the structure formation, domain sizes and domain distances. UV-Vis and Pl are used to analyze differences in the optical properties of the thin films. These structural and optical changes are then correlated with measurements of the Seebeck coefficient and the electrical conductivity.

CPP 35.3 Wed 11:00 P1

A two-state Gaussian loop under tension: negative extensibility and ensemble inequivalence — •Geunho Noh and Panayotis Benetatos — Department of Physics, Kyungpook National University, Republic of Korea

Loop formation is commonly observed in biopolymers and, in many cases, the loop structure is transient. Some examples of this structural rearrangement are the formation of denaturation bubbles in double-stranded DNA and the transient DNA looping associated with gene regulation. Here, we study the conformational statistics and the elastic behavior of a flexible polymer under tension with a two-state structure: looped or unlooped. We analyze two cases. In the first, the loop can zip to form a double-stranded chain. In the second, the dangling ends of a chain can bind to form a loop. In each case, we investigate the force-extension relation of the two-state loop in both the Helmholtz and the Gibbs ensembles. We also extend the two-level system to a three-level Gaussian loop by introducing a third (intermediate) state. In contrast to the single Gaussian chain, the two- or three-level systems show qualitatively different tensile response and ensemble inequivalence. Interestingly they can have negative extensibility in the Helmholtz ensemble, and we point out that this is one of the simplest polymer models which exhibits such metamaterial-like behavior.

CPP 35.4 Wed 11:00 P1

Determination of the roast-dependent pore size in coffee beans using positron lifetime spectroscopy — •Adrian Langrehr, Vassily Burwitz, Lucian Mathes, and Christoph Hugenschmidt — Forschungs-Neutronenquelle Heinz Maier-Leibnitz (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Positron Annihilation Lifetime Spectroscopy (PALS) is an established method to determine the type and concentration of open volume defects in crystals as well as to investigate the free volume in polymers. Using ^{22}Na as β^+emitting radioisotope in the so-called "sandwich" geometry we present the capabilities of our four-detector setup with digital readout and signal processing. The efficient readout of this PAL spectrometer produces 12 lifetime spectra simultaneously. Our study encompasses the comparison of three different methods to combine information contained in these 12 spectra. To demonstrate a use case of a biomaterial we measured the positron lifetimes in coffee beans as a function of the degree of roasting. The application of the so-called Tao-Eldrup model allows us to study the influence of the roasting parameters on the mean pore size on the nanometer scale.

CPP 35.5 Wed 11:00 P1

Microgels for Enhanced Adsorption of Endothelial Cells on Artificial Networks — •Souraj Mandal and Regine von Klitzing — Soft Matter at Interfaces, Department of Physics, Technical University of Darmstadt, Germany

Artificial 3-D supply networks can be applied as a transport system for oxygen and nutrients, which can promote vascularization for organ-like 3-D cell culture systems. In the human body, the inner surface of such networks (blood vessels) is lined with a layer of endothelial cells and they play a vital role in cell maturation and angiogenesis (formation of new blood vessels). So far, the attachment of endothelial cells on the surface of the artificial network system is not sufficient. Addressing this problem, this study focuses on designing a suitable mediator between the inner walls of the artificial network and endothelial cells, which should be mechanically stable to flows of nutrient solutions. Here we employ Poly(N-isopropylacrylamide) (PNIPAm) microgel (MG) as cell-culturing surface mediator. However, the main challenges are (i) ensuring the firm adhesion of MGs on the surface of the artificial polymeric network, and (ii) seeding endothelial cells on top of them. As a primary approach, we synthesized positively charged MGs to attach them on plasma-treated silicon (Si) and 3-D printed polymeric surfaces. MG particles are characterized by their Zeta potential and hydrodynamic radius. As a rapid fabrication technique, spin coating was used to deposit a thin polymeric layer of MG particles on the substrates. AFM analyses showed a stable adhesion of MG particles on the flat surfaces even upon water washing and mechanical stress.

CPP 35.6 Wed 11:00 P1

Depletion induced phase behavior and equilibrium clusters in charged BSA and HSA protein solutions — •Maximilian D. Senft, Fajun Zhang, and Frank Schreiber — Universität Tübingen, Germany

Understanding and predicting the phase behavior of proteins is an ongoing endeavor in many scientific research areas, including the pharmaceutical industry. In addition to crystallization, liquid-liquid phase separation and condensate formation, which includes equilibrium clusters, dense liquid droplets, fibrils, and gels, appear to be closely related to many pathological conditions. The formation of equilibrium protein clusters in solution requires an interaction potential with competing contributions, i.e., long-ranged repulsion and short ranged attraction. Bovine and human serum albumin (BSA and HSA) carry negative charges at neutral pH which provide a long-range electrostatic repulsion between proteins. The attractive potential can be generated via the depletion interactions introduced by the non-adsorbing polymer polyethylene glycol in protein solutions. By tuning the ionic strength, polymer size and concentration, the competing potential can be continuously adjusted, resulting in equilibrium protein clusters due to the subtle balance to the different contributions of the interaction potential. Having performed systematic small angle scattering measurements, on BSA and HSA, together with quantitative modeling combined with protein phase diagrams a better understanding of depletion induced protein phase behavior and cluster state can be provided.

CPP 35.7 Wed 11:00 P1

Purely elastic instability of semi-dilute polymer solutions in shear flow — Pegah Shakeri[1,2], •Michael Jung[1,2], and Ralf Seemann[1,2] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Max Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

Polymer solutions in the semi-dilute regime are of considerable industrial importance. The complex rheological properties of such highly viscoelastic fluids and the complexity of their flow characteristics, especially in curved geometries, require a thorough experimental characterization of the dynamics of such fluid flows. We experimentally investigate the flow of highly elastic polymer solutions above their overlap concentrations in a microfluidic serpentine channel using pressure measurements and particle image velocimetry. Our results show that the flow resistance increases significantly at high Weissenberg numbers but vanishing Reynolds numbers, indicating the occurrence of a purely elastic instability. We show that the onset of instability can be scaled by including shear-dependent rheological properties of the polymer solutions in the nonlinear stability analysis. As a result, a universal criterion as a function of normalized polymer concentration is provided for scaling the onset of pure elastic instability in the semi-dilute regime independent of the type and molecular weight of the polymer.

CPP 35.8 Wed 11:00 P1

Improved displacement efficiency in porous media by invasion of viscoelastic fluids — •Michael Jung[1,2], Pegah Shakeri[1,2], and Ralf Seemann[1,2] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Max Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

Improving the displacement efficiency of capillary entrapments in porous media by adding high molecular weight polymers to the invading phase has a variety of industrial applications. Apart from an increased viscosity contrast compared to water flooding, the flow of viscoelastic polymer solutions exhibits unstable flow behavior even at small Reynolds numbers, which can lead to an additional displacement mechanism of the capillary entrapments. We use a microfluidic approach to reveal the underlying mechanism of this enhanced displacement by first considering a random array of cylindrical posts to identify fundamental differences in displacement processes for elastic and non-elastic fluids. Then, to focus directly on displacement processes driven solely by elastic stresses and to exclude the effects of viscous stresses, we consider a single capillary entrapment connected to two symmetric serpentine channels. We show that the unique viscoelastic fluid features, such as the emergence of a significant first normal stress difference, combined with the curved flow geometry, lead to purely elastic instability and elastic secondary flow, which in turn generate the stresses required to overcome the capillary threshold and displace capillary entrapment.

CPP 35.9 Wed 11:00 P1

Supraparticles: Aggregation of colloids in evaporating dispersion drops — •Melis Yetkin[1], Yashraj Manish Wani[2], Arash Nikoubashman[2], Michael Kappl[1], and Hans-Jürgen Butt[1] — [1]Department of Physics at Interfaces, Max-Planck-Institute for Polymer Research, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz,Germany

Evaporating dispersion drops from superamphiphobic surfaces opens a way to fabricate supraparticles (SPs) with complex structures. The structure formation can be controlled by tailoring the interaction forces between particles and process conditions. In this study, the structure of the SPs was investigated by tuning the shape of the primary building blocks and the process conditions. Ellipsoidal polystyrene (PS) particles of different aspect ratios were obtained by stretching a polymeric film of spherical particles above the glass transition temperature. Aqueous dispersion drops of the ellipsodal particles were evaporated from silicone nanofilaments-based superamphiphobic surfaces under varying humidity conditions, during which the evaporation process was monitored by a camera. The interaction between the building blocks, and hence the final morphology of the SPs, were altered by the addition of surfactant sodium dodecyl sulfate (SDS). Control experiments with spherical PS building blocks were conducted in parallel. The study elucidated the effect of primary building block shape on the final morphology of supraparticles and the transition between a shape-dominated regime and an interaction-dominated regime.

CPP 35.10 Wed 11:00 P1

Temperature dependent measurments of the diffusion- and Soret-coefficient in a binary polystyrene/toluene mixture — •Jannik Kantelhardt and Werner Köhler — Physikalisches Institut Universität Bayreuth, Germany

In this work we investigate the dependence of the diffusion- and Soret-coefficient in respect to different ambient temperatures with a temperature range from 10°C to 50°C in steps of 5°C. The here investigated system, a solution of polystyrene (PS) in toluene with a weight fraction of c_{PS}=1%, has in a similar concentration also been used in the binary companion cell of the DCMIX4 microgravity campaign on ternary mixtures. Furthermore, binary and ternary polystyrene solutions are candidates for the forthcoming GIANT FLUCTATIONS project of ESA for the investigation of non-equilibrium fluctuations under microgravity conditions.

The measuements were performed with a Thermal-Diffusion-Forced-Rayleigh-Scattering (TDFRS) setup. Through a writing beam a holographic grating is created inside the mixture where a small amount of an inert dye is added. The grating heats the sample periodically which leads to temperature gradients. Through the Soret-effect concentration gradients appear and both lead to changes in the refractive index. The signal is measured with a readout beam under Bragg diffraction.

CPP 35.11 Wed 11:00 P1

Diffusion, Thermodiffusion and turbidity of thermoresponsive Poly(N-acryloylglycinamide) in water. — •Roman Reh[1], Nikola Majstorovic[2], Seema Agarwal[2], and Werner Köhler[1] — [1]Universität Bayreuth, Physikalisches Institut, Germany — [2]Universität Bayreuth, Macromolecular Chemistry II, Germany

We report about measurements on Poly(N-acryloylglycinamide) (PNAGA) in aqueous solution. Diffusion-, Thermodiffusion- and Soretcoefficients were measured with the polymer in linear form and as a crosslinked microgel. Furthermore, temperature dependent measurements on turbidity were done with the linear polymer. Experiments on diffusion were performed with the Optical-Beam-Deflection technique where a vertical temperature gradient is applied to the sample and information about the time dependent distribution of temperature and concentration in the sample is gathered by recording the position of a laser beam, which traverses the sample and gets deflected. This is because the refractive index changes with temperature and concentration, which on its part changes due to thermodiffusion. Turbidity measurments show a UCST-behavior and a hysteresis in the temperature of the cloud point, depending on the direction of the temperature ramp, which is in accordance with results from literature. Thermodiffiusion- and Soretcoefficients at different temperatures are described with an exponential Piazza function [S. Iacopini et al., Eur. Phys. J. E **19**, 59-67 (2006)] and are comparable for the linear polymer and the microgel, showing a systematical behaviour and a change in sign in the region of about 35 to 40 °C.

CPP 35.12 Wed 11:00 P1

Measurement of diffusion and thermodiffusion of polydisperse polymers by means of a compact optical beam deflection setup — •Mareike Hager, Roman Reh, and Werner Köhler — Universität Bayreuth, Physikalisches Institut, Germany

We have performed diffusion and thermodiffusion experiments on solutions of polydisperse polymers by means of a newly developed double-pass optical beam deflection (OBD) instrument. The aim is to develop a model for the description of the multimodal OBD signals and to develop the technique into a method for polydispersity analysis. The double-pass OBD instrument utilizes a laser beam that is reflected behind the Soret cell and passes the sample volume a second time. In the cell a vertical temperature gradient is applied that leads to thermodiffusion in the sample and, thus, to a concentration gradient and a gradient of the refractive index. The laser beam that traverses the cell twice is deflected and detected on a camera where the time dependent laser position is recorded. From the measured OBD signal the diffusion, thermodiffusion and Soret coefficients can be extracted. The multimodal time traces are evaluated with an adapted version of the CONTIN program for the solution of inverse problems. It is shown that diffusion coefficients extracted in this way agree with literature data. The results of the measurements of samples with two polymers of different sizes are in accordance with the results for the single components. Based on these results, polymers with a broad molar mass distribution can now be investigated.

CPP 35.13 Wed 11:00 P1

Mixture of magnetic and non-magnetic ellipsoids — •Elena Pyanzina[1], Anna Akisheva[1], Tatyana Belayeva[1], Marina Gupalo[1], and Sofia Kantorovich[2] — [1]Ekaterinburg, Russia — [2]University of Vienna, Vienna, Austria

In this contribution, mixtures of magnetic and non-magnetic ellipsoids were studied. We chose systems with the ratio of the semi-axes equal to 3 and 5 and different concentrations, as well as the direction of the magnetic moment along the main axis. The ratios of magnetic and non-magnetic particles considered were as follows: 30/70, 50/50 and 70/30. The initial susceptibility of such systems was calculated since the magnetic response of the system is very important for various applications. It turned out that with an increase in the magnitude of the magnetic moment, a structural transition occurs in the system: first, the initial susceptibility increases, and then it becomes almost zero. This is because the basic state of elongated ellipsoids is an antiparallel pair, which becomes stable with an increase in the magnitude of the magnetic moment. And its total magnetic moment is quite small, and the susceptibility of such an object is much lower than that of a pair of particles with a head to tail orientation. The behavior of mixtures of ellipsoids with similar systems of magnetic disks (like ellipsoids with a magnetic moment perpendicular to the main axis) was also compared. It turned out that at large values of the magnetic moment, the disks form "stacks" in which the magnetic moments are directed head to tail, and ellipsoids form flat structures with a thickness of one ellipsoid, with an antiparallel orientation of the moments.

CPP 35.14 Wed 11:00 P1

Mesoporous polymers as electrode material in hybrid organic-inorganic lithium-ion batteries — •Tom Wickenhäuser[1], Lucas Ueberricke[2], Angelina Jocic[2], Erik Misselwitz[2], Elisa Thauer[1], Yuquan Wu[1], Michael Mastalerz[2], Milan Kivala[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Institute of Organic Chemistry, Heidelberg University, Germany

We report on the characterisation of mesoporous polymers as electrode materials in hybrid organic-inorganic lithium-ion batteries. In particular, dendritic pyrene tetraone (D-PTO) and triphenylamine (TPA) is investigated as cathode material and non-planar covalent carbon networks are studied as anode material in lithium half-cells. Cyclic voltammetry as well as galvanostatic cycling measurements were done to investigate on ionic and electric transport mechanisms. For redox active dendritic pyrene tetraone, the mesoporous character of the amorphous polymer is confirmed and the specific surface areas range up to nearly 700 m^2g^{-1}. Galvanostatic cycling measurements show a specific capacity of 137 $mAhg^{-1}$ and a capacity retention of 86% after 50 cycles.

CPP 35.15 Wed 11:00 P1

Design, fabrication and nano-scale characterization of novel SEI layers — •Zhuijun Xu[1], Yajun Cheng[2], Yonggao Xia[2], and Peter Müller-Buschbaum[1,3] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, 315201, Ningbo, China — [3]MLZ, TUM, 85748 Garching, Germany

Rechargeable lithium metal batteries have been recognized as one of the most promising energy storage devices due to their superior energy density. However, serious safety concerns and poor cyclability are challenges originating from an uncontrolled lithium dendrite growth and an unstable solid electrolyte interface (SEI) layer. SEI can be enhanced by synergetic additives in commercial electrolytes. Herein, amphiphilic block copolymers/inorganic materials–PS-b-PEO/LiNO3 as additives, which bear some clear advantages including absorbing mechanical stress, conducting lithium ion and controlling the lithium dendrite growth, are mixed with commercial electrolytes and applied in the lithium metal battery. Remarkably, Li symmetric cells have a long-term cycling life over 300 h with a capacity of 3 mAh cm-2. Moreover, full battery with lithium metal anode and LiFePO4 exhibits a stable and high capacity of 138 mAh g-1 at 1 C. With ex-situ scattering techniques or in-situ scattering studies, the structures of the surface modified lithium metal anodes and structure formation processes are studied.

CPP 35.16 Wed 11:00 P1

Less is more: tiny amounts of insoluble multi-functional microporous additive plays a big role in lithium secondary batteries — •Ruoxuan Qi[1], Peter Müller-Buschbaum[1,2], and Yajun Cheng[3] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]MLZ, TUM, Garching, Germany — [3]NIMTE, CAS, Zhejiang Province, P. R. China

Binders play an important role in multi-component electrodes for rechargeable batteries, which suffer from poor electronic and ionic conductivity. Binder-free electrodes provide another way to resolve problems, where sophisticated structure construction is required. A new concept of electrode processing alternative to binder-containing and binder-free electrodes was established. A multi-functional PIM-1 (a polymer with intrinsic microporosity) additive was used instead of PVDF to form mechanically processable Li secondary battery cathodes. Due to its unique nanoporous structure built by the spiro-containing rigid aromatic polymer chain, only a tiny amount of PIM-1 in the LiNi0.8Co0.1Mn0.1O2 cathode is needed to retain good performance, far below the typical composition for PVDF. Homogeneous dispersion of carbon black is achieved by PIM-1, which stabilizes the electrode and increases the electronic conductivity. Different from PVDF, mechanical buffering by stiff PIM-1 yields crack-free electrodes after cycles. Moreover, an inorganic rich cathode-electrolyte interface layer is formed via a desolvation process promoted by PIM-1, because of its strong binding ability with lithium ions, which is beneficial for cyclic stability and rate capability.

CPP 35.17 Wed 11:00 P1

Positrons probe advanced and functionalized porous materials — •Ahmed Gamal Attallah, Eric Hirschmann, Maik Butterling, Maciej Oskar Liedke, and Andreas Wagner — Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf

Positron annihilation lifetime spectroscopy (PALS) is an effective porosimetry technique complementing standard gas intrusion methods. PALS is able to detect open and closed pores, and resolve depth-dependent porosity. It can operate under variable pressures, temperatures, and atmospheres to monitor structural changes during in situ conditions. In this contribution, PALS results of various functionalized porous materials including polymer grating, structural changes in metal-organic-frameworks (MOFs), effect of additives in food ingredients (maltodextrin) on water uptake, and impact of modification of low-k dielectrics on stiffness will be presented. In polymer grafting, the mechanism of polymer grafting on MCM-48-type mesoporous silica nanoparticles forming core-shell composite structure is understood from PALS. Uniquely in MOFs, PALS was able to prove that the temperature-driven transformed metal-organic framework DUT-8(Ni) is still porous possessing closed porosity that is not accessible by other techniques. Sucrose in maltodextrin is the third topic where in situ humidity experiment during PALS revealed that adding 10 % sucrose to maltodextrins has a negligible effect on hygrocapacity at relative humidity > 50 %. Finally, the improved mechanical stability of low-k materials by adding methyl terminal groups that cause less interconnected pores has been verified by positron annihilation.

CPP 35.18 Wed 11:00 P1

Insights into the morphology-structure-property relationship of mesoporous ZnO films during humidity sensing — •Ting Tian[1], Shanshan Yin[1], Suo Tu[1], Apostolos Vagias[2], Anna-Lena Oechsle[1], Tianxiao Xiao[1], Sigrid Bernstorff[3], and Peter Müller-Buschbaum[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, 85748 Garching — [2]MLZ, TU München, 85748 Garching — [3]Elettra-Sincrotrone Trieste S.C.p.A., Strada Statale 14 km 163.5, AREA Science Park, Basovizza, 34149 Trieste, Italy

Moisture can strongly influence the conductivity of ZnO semiconductors via the physisorption and chemisorption of water molecules on the ZnO surface. Mesoporous ZnO structures can facilitate the absorption process by providing a large surface area and active sites. However, little effort has been devoted yet to gain an in-depth understanding of the effect of water on the morphology and electrical property In the present work, different mesoporous ZnO thin films were synthesized by exploiting different diblock copolymers. Benefiting from the different inorganic frameworks, these thin films show significantly different structural properties and defects density. To explore the morphology-structure-property relationship, in situ Fourier-transform infrared spectroscopy (FTIR) was used to confirm the water absorption. Simutalenouesly, in situ grazing-incidence small-angle X-ray scattering (GISAXS) measurements were performed to investigate the morphology evolution, and in situ electrochemical impedance spectroscopy (EIS) was used to monitor the conductivity changes.

CPP 35.19 Wed 11:00 P1

Morphology transformation pathway of block copolymer-directed cooperative self-assembly of ZnO hybrid films monitored in situ during slot-die coating — •Ting Tian[1], Shanshan Yin[1], Suo Tu[1], Christian L. Weindl[1], Kerstin S. Wienhold[1], Suzhe Liang[1], Matthias Schwartzkopf[2], Stephan Volkher Roth[2], and Peter Müller-Buschbaum[1,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, 85748 Garching — [2]James-Franck-Str. 1 — [3]MLZ, TUM, 85748 Garching

Co-assembly of diblock copolymers (DBCs) and inorganic precursors that takes inspiration from the rich phase separation behavior of DBCs can enable the realization of a broad spectrum of functional nanostructures with the desired sizes. In a DBC assisted sol*gel chemistry approach with polystyrene-block-poly(ethylene oxide) and ZnO, hybrid films are formed with slot-die coating. Pure DBC films are printed as control. In situ grazing-incidence small-angle X-ray scattering (GISAXS) measurements are performed to investigate the self-assembly and co-assembly process during the film formation. Combining complementary ex situ characterizations, several distinct regimes are differentiated to describe the morphological transformations from the initially solvent-dispersed to the ultimately solidified films. The precursor reduces the degree of order, prevents crystallization of the poly(ethylene oxide) block, and introduces additional length scales in the hybrid films.

CPP 35.20 Wed 11:00 P1

Evaluation of different textile mount designs for printing on textiles in commercial SLA 3D printers for scientific investigation — •Timo Grothe[1], Elise Diestelhorst[1], Jan Lukas Storck[1], Daniel Koske[1], Natalie Frese[2], and Martin Wortmann[2] — [1]Faculty of Engineering and Mathematics, Bielefeld University of Applied Sciences, Interaktion 1,33619 Bielefeld, Germany — [2]Faculty of Physics, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany

The technology of 3D printing has already reached the commercial sector. But it is not only the industry that is interested in 3D printing; the scientific world is also investigating the possibilities of this multifaceted technology. Here, in addition to the fused deposition modeling (FDM) process, the cornerstone stereolithographic (SLA) process in particular has become the focus of scientific attention. Especially in combination with textiles, some unique composites with outstanding properties can be produced. In order to be able to print these in commercially available printers, some textile mounts were developed and their applicability as well as usability were investigated. Not only the printing result and the adhesion between resin and different textiles were investigated by abrasion tests, but also the application of the individual holders was evaluated. Finally, the produced composites were examined with a scanning helium ion microscope to show, in combination with the other examination methods, that both the textile-resin composites have exceptional abrasion resistance and that the textile holders make it much easier to produce them.

CPP 35.21 Wed 11:00 P1

Polymer Composite Films with Induced Structural Anisotropy for Thermoelectric Application — •Christian Gradl[1], Marie Siegert[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

Thermoelectric generators offer a prospective opportunity to handle the increasing energy demand by utilizing waste heat. Organic thin films represent a promising candidate because of benefits like non-toxicity, cost-effectivity or versatile implementation. For an efficient thermoelectric device, the thermoelectric figure of merit $zT = \sigma S^2 T/\kappa$ needs to be high. So the Seebeck coefficient S and the electrical conductivity σ should achieve high values, whereas the thermal conductivity κ has to be low. Taking advantage of the intrinsically low κ, we combine the polymer PEDOT:PSS with additives like silver nanowires, the crystalline organic TTT_2I_3 or VO_2 needles, by which a higher σ is aspired without pronounced detriment of the Seebeck coefficient. TTT_2I_3 and VO_2 are fabricated via microspacing in-air sublimation. Controlled orientation of the additives induced by the substrate is a main topic of our research. Further we investigate the alignment of additives embedded in polymer thin films prepared via doctor-blading to improve the efficiency for thermoelectric application. The results on characterizing the electrical and thermal properties of the organic-metallic composites with respect to their anisotropy will be presented.

CPP 35.22 Wed 11:00 P1

Morphological studies in semicrystalline polymers and polymer nanocomposites using spin diffusion — •Dorit Hartmann, Anna Nitsche, Yury Golitsyn, Horst Schneider, and Kay Saalwächter — Department of Physics / NMR Group, University of Halle, Betty-Heimann-Str. 7, 06120 Halle, Germany

ABSTRACT: The properties of synthetic polymers can be selectively modified by adding nanoparticles, which is why polymer nanocomposites have a wide range of applications. The interaction of the polymer chains with the surface of silica particles leads to the formation of a multiphase structure, characterized by a gradient of molecular dynamics. [1] Studies of polymer nanocomposites using spin diffusion (SD) experiments in conjunction with the numerical simulations have shown that the interphases exhibit complex morphology with dynamic heterogeneities. [2] In this work, we investigate the effect of magnetic field strength on spin diffusion in semicrystalline poly(ϵ-caprolactone) and a poly(2-vinyl pyridine)-silica nanocomposite. The experiments were performed at two different field strengths of 0.47 T and 4.7 T (proton Larmor frequency of 20 MHz and 200 MHz, respectively) and were supported by spin diffusion calculations. In addition, this paper aims to provide an overview of the different data acquisition and analysis strategies for high- and low-field instruments. REFERENCES: [1] Horst Schneider, Kay Saalwächter, and Matthias Roos. Macromol. (2017), 50, 8598-8610. [2] Horst Schneider, Matthias Roos, Yury Golitsyn, Kerstin Steiner, and Kay Saalwächter. Macromol. Rapid Commun. (2021), 2100061.

CPP 35.23 Wed 11:00 P1

Two-step electrochemical Au nanoparticle formation in polyaniline — •Bin Zhao and Sebastian Gutsch — institut für mikrosystemtechnik, freiburg, germany

In this study, we report on an electrochemical insertion of Au nanoparticles in polyaniline (PANI) using a two-step process. In the first step, tetrachloroaurate anions (AuCl4-) are attached on the protonated imine sites of PANI while holding the potential at +0.8 V. The applied electrochemical potential prevents any reduction of the PANI/AuCl4- complex. After rinsing of excess AuCl4-, a controlled reduction is carried out via cyclic voltammetry. Therefore, we investigate the introduction of Au species into PANI via precise electrochemical control in a flow cell system. The PANI/Au composites are characterized using scanning electron microscopy (SEM) and Rutherford backscattering spectrometry (RBS) to quantify the amount of introduced Au. It is demonstrated that the PANI/AuCl4- complex is not aggregating prior to the electrochemical reduction process. However, the controlled reduction of these PANI/Au complexes leads to the subsequent formation of Au nanoparticles, whose density and size dispersion depend on the Au loading in PANI. Furthermore, additional Au deposition cycles increase both the Au nanoparticle density and size. We propose a two-step growth model based on our experimental results. The results are discussed with respect to the formation of atomic Au clusters reported in previous works.

CPP 35.24 Wed 11:00 P1

Accelerating self-assembly of colloidal particles at air-water interface by laser induced heating of upconverting particle — •Lokesh Chinnakanna Muruga, Gokul Nalupurackal, Sresta Roy, Snigdhadev Chakraborty, Jayesh Goswami, and Basudev Roy — Indian Institute of Technology Madras, Chennai, India -

600036

Particles can be assembled at the air-water interface due to optically induced local heating. This induces convection currents in the water which brings particles to the surface. We improve the technique by employing an upconverting particle (UCP), which, when illuminated with 975 nm light, not only emits visible emission but also generates heat owing to the poor efficiency of the upconversion process. This induces strong convection currents which makes particles dispersed in the suspension assemble at the interface and immediately under the UCP. We show assembly of polystyrene particles of 1 μm diameter and diamonds of 500 nm diameter bearing Nitrogen-Vacancy (NV) centers around the UCP. We also show, for the first time, that the microdiamonds are assembled within about 30 nm at the bottom of the UCP by utilizing non-radiative energy transfer that reduces the lifetime of the 550 nm emission from about 90 μs to about 50 μs.

CPP 35.25 Wed 11:00 P1

Following the directed self-assembly of crystallizable block co oligmers via in situ AFM — •Alexander Meinhardt[1], Peng Qi[2], Ivan Maximov[3], and Thomas F. Keller[1] — [1]Centre for X-ray and Nano Science (CXNS), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Paul Scherrer Institut, Villigen, Switzerland — [3]Solid State Physics and NanoLund, Lund University, Lund, Sweden

Bottom up nanofabrication utilizing the molecular self-assembly of block co-oligomers with sub-10 nm domain sizes is widely discussed as a promising route for next generation photolithography. Double crystalline co-oligomers can be used to create well defined, high-fidelity nanostructures by controlling the competing driving forces microphase separation and crystallization. We report on the surface nanostructure formation and the temporal evolution during annealing of thin films of an amphiphilic double crystalline polyethylene-block-poly(ethylene oxide) co-oligomer (PE-b-PEO) on planar and patterned surfaces. On a planar Si surface we observed the self-assembly of PE-b-PEO into locally ordered lamellar surface structures extending over several micrometers. Directed self-assembly (DSA) of this PE-b-PEO system by physical guiding patterns can enable the formation of large scale nanotemplates interesting for future applications. First DSA experiments indicate that the formed PE-b-PEO based surface nanostructures depend on the pitch of the guiding pattern. We furthermore aim to use in situ AFM to shed light on the pitch-dependent structural evolution during dedicated temperature-controlled annealing procedures.

CPP 35.26 Wed 11:00 P1

Intracrystalline dynamics of polybutylene succinate and poly(3-Hydroxybutyrate) — •Mohd Afiq Bin Anuar, Yu Qiang, Thomas Thurn-Albrecht, and Kay Saalwächter — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany

The dynamics behavior of polymers chain in crystal lamellae plays a critical role for its semicrystalline morphology [1, 2]. It is influenced by this intracrystalline dynamics (ICD) explaining the factors that limit its crystal thickness during isothermal crystallization. In this work, two different behaviours of semicrystalline polyesters, namely polybutylene succinate (PBS) and poly(3-Hydroxybutyrate) (P3HB), are discussed. A combination of nuclear magnetic resonance (NMR) techniques shows that isothermally crystallized PBS exhibit slow ICD longer than 1s which is similar to the reported crystal-fixed polymer, polycaprolactone [1]. Meanwhile, in P3HB crystal chain, the ICD with correlation jump motion around 0.5s/monomer at 120°C was detected. This is in contrast to previous reported [3] demonstrating a crystal-mobile behavior. Small-angle X-ray scattering measurement reveal that the P3HB crystal lamellae are significantly thicker than in PBS, confirming that P3HB and PBS can be classified as crystal-mobile and crystal-fixed, respectively. Details regarding morphology are shown in the poster.

References: [1] Schulz, M., et al., Macromolecules 2018, 51, 8377. [2] Schulz, M., et al., Nat. Common. 2022, 13, 1. [3] Xia, Z., et al., Soft Matter 2021, 17, 4195.

CPP 35.27 Wed 11:00 P1

Non-linear mechanical properties of polycaprolactone polymer/oligomer blends with defined entanglement density and crystalline thickness — •Tonghua Liu, Albrecht Petzold, and Thomas Thurn-Albrecht — Von-Danckelmann-Platz 3, 06120, Halle(Saale)

The mechanical properties of semi-crystalline polymers are determined by the semi-crystalline morphology and the entanglements in the amorphous regions. Here we use polymer/oligomer blends to control the entanglement density independently of the crystallinity. This system is also used as a model to study effects on the non-linear mechanical properties. The aim of the project is to develop a quantitative method for the determination of the entanglement density in the amorphous region as well as to investigate its relation to yielding, modulus and strain hardening. The commonly used method is tensile testing, but cavitation and necking cannot be avoided. Instead, we use plane-strain compression tests, which allow the direct determination of the true stress and avoids problems like cavitation. A separation of viscous and elastic contributions can be achieved by inserting relaxation measurements during the deformation. Our preliminary results indicate a strong effect of the crystallinity on the modulus and yield stress. The relation between strain hardening and entanglement density will be discussed.

CPP 35.28 Wed 11:00 P1

New experimental methods for structure analysis of soft matter — •Eric Euchler[1], Anna Katharina Sambale[1], Regine Boldt[1], Kai Uhlig[1], Laura Neumann[1], Konrad Schneider[1], Matthias Schwartzkopf[2], Stephan Roth[2,3], and Markus Stommel[1,4] — [1]Leibniz-Institut fuer Polymerforschung, Dresden, Germany — [2]Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — [3]KTH Royal Institute of Technology, Stockholm, Sweden — [4]Technical University Dresden, Dresden, Germany

Recently developed stretching devices for synchrotron measurements are available to investigate deformation-induced phenomena, such as strain-induced crystallization in natural rubber or void formation in biological tissues, at quasi-static and impact loading. In addition to measurements in transmission, novel studies of thin layers on flexible substrates can be realized by performing in situ grazing-incidence (GI) experiments.

Beside structure analysis in solid parts, the flow-induced structure formation in polymer melts is of particular interest to better understand the impact of melt processing parameters on macroscopic material properties, such as Young's modulus and tensile strength. For this purpose, a new experimental setup has been designed and built to study time- and temperature-dependent structure evolution events in thermoplastics. Within a temperature-controlled flow channel, polymer melts can be monitored with a microfocus X-ray synchrotron beam and first results obtained for two different thermoplastic materials proofed the experimental concept under quiescent melt conditions.

CPP 35.29 Wed 11:00 P1

Towards experimental detection of crystallization in individualized polymer chains — •Wing Kit Or, Alaa Hassan, and Martin Tress — Peter Debye Institute for Soft Matter Physics, Leipzig University, Leipzig, Germany

Although crystallization of polymers has been investigated since decades, it is not yet fully understood. One way to gain more insight is to study the difference between bulk polymer and confined polymer chains with focus on how crystallization characteristics change depending on the size and type of confinement. Until now, most studies have used confinement in thin films or nanopores but the approach to study crystallization and aggregation in individual chains was accessible only to computer simulations. Since detection of phase transitions in individual polymer chains poses a severe challenge to most experimental methods, the measurement of ensembles of individual chains is desirable. However, maintaining the individual character requires a sophisticated method to separate them. Here, we use block copolymer micelle lithography (BCML) to deposit a regular pattern of well-separated gold nanodots on a silicon substrate in order to chemically graft end-functionalized polymer chains on these nanodots to individualize them. Instead of common thermodynamic methods (which require considerably more sample material), we employ dielectric spectroscopy using a nanostructured electrode arrangement since it is much more sensitive. Albeit being typically considered a dynamics method, it also allows to examine density changes and thus phase transitions of polymers.

CPP 35.30 Wed 11:00 P1

Uniaxially Aligned Merocyanine Films by Graphene Nanoribbon Templated Growth — •Philipp Weitkamp, Nora Gildemeister, Lukas Böhner, Dirk Hertel, and Klaus Meerholz — Physikalische Chemie, Universität zu Köln, Deutschland

We herein report the unique and novel approach of achieving a polycrystalline thin film consisting of uniaxially aligned domains by using 7-armchair graphene nanoribbon (7-aGNR) monolayers as van-der-Waals template. For this purpose, a merocyanine dye was evaporated on 7-aGNRs, transferred on quartz glass substrates. The alignment of the formed molecular aggregate along the GNR alignment direction was proven by polarisation dependent absorbance spectroscopy. The J- and H-transition, formed by the dye aggregate, were correlated with distinct axes of the crystal structure. By combining this correlation with polarisation dependent absorbance measurements and X-ray diffraction experiments we elucidated the three-dimensional structure of the formed aggregate thin film. The growth mode of these films was investigated as a function of the applied layer thickness. Atomic force microscopy-based morphology analysis and X-ray diffraction experiments were used to reveal the anisotropic on-surface crystallisation along the 7-aGNR long axes direction. Furthermore, we found that the delocalisation length of the aggregate increases with increasing in-plane order. Finally, we demonstrated that the in-plane alignment leads to an anisotropic charge carrier transport by implementing the templated merocyanine thin film as active layer in a top-gated organic field effect transistor.

CPP 35.31 Wed 11:00 P1

Long chain Polyamides: Influence of methylene sequence length and external forces on structural features — •Rene Sattler[1,2], Varun Danke[3], and Mario Beiner[1,2] — [1]Fraunhofer IMWS, Walter-Hülse-Str. 1, D-06120 Halle (Saale), — [2]Martin-Luther-Universität Halle-Wittenberg, Naturwissenschaftliche Fakultät II, D-06099 Halle (Saale) — [3]Evonik Operations GmbH, Research Development & Innovation, Paul-Baumann-Str. 1, D-45722 Marl

Crystallographic studies towards the influence of methylene sequence length on a series of even-even polyamides PA 10.n (with n = 12, 14, 16 and 18) are performed. Temperature-dependent X-ray diffraction measurements show that the triclinic α phase is the preferred phase at room temperature after slow cooling from melt. In PA 10.12 and PA 10.14 a reversible Brill transition to the (pseudo)hexagonal high temperature γ phase is observed. However, the Brill transition temperature is strongly dependent on n and shifting to higher temperatures with increasing methylene sequence length. For the two higher members a Brill transition is absent. The analysis of annealed, uniaxial oriented fibers reveals that the crystalline state achieved under ambient conditions is influenced by external forces. This is due to relatively small energetic differences between the α and β polymorphs. All the uniaxial oriented PA 10.n samples show a β polymorph which is most prominent for PA 10.12 and PA 10.14. The higher members show a mixture of the β polymorph superimposed with a certain franction of the α polymorph.

CPP 35.32 Wed 11:00 P1

Bond order parameters in crystallization of short polymer chains in thin films: SAMC simulation — •Evgeniia Filimonova, Timur Shakirov, and Viktor Ivanov — Martin Luther University of Halle-Wittenberg, Institute of Physics, 06120, Halle (Saale), Germany

We study the crystallization of polymer melts in thin films using a coarse-grained model and stochastic approximation Monte Carlo (SAMC) simulation. Our goal is to reveal physical factors which are responsible for one of two possible scenarios of surface-induced polymer crystallization: heterogeneous nucleation or prefreezing. We have developed an approach that allows us to identify the translational and orientational local ordering by means of comparing our system configurations with reference crystalline structures of different symmetries. In addition to calculating the usual order parameters (Steinhardt parameters, common neighbors analysis, nematic order parameter, etc.), we suggested new order parameters based on scalar products of bonds between nearest neighbors. We observe a coexistence of an isotopic structure in the center of the film with ordered structures at the walls at intermediate values of energies (in microcanonical analysis). A change in the crystal structure accompanying a change in density at different energies is also shown. Financial support of the International Graduate School AGRIPOLY supported by the European Social Fund (ESF) and the Federal State Saxony-Anhalt is acknowledged.

CPP 35.33 Wed 11:00 P1

Investigating the thermodynamics and kinetics of catechin pyrolysis for environmentally friendly binders — •Jakob Kraus and Jens Kortus — Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Str. 23, D-09599 Freiberg, Germany

The thermodynamics and kinetics of the pyrolysis of (+)-catechin, a building block of the condensed tannins found in recipes for sustainable binders, are evaluated at the CCSD(T) level and compared to other methods from quantum chemistry. Using the climbing image nudged elastic band method coupled with transition state optimization, minimum energy paths and highest-energy transition states are identified for the first two pyrolysis steps, a catechol splitoff with subsequent dehydrogenation. While the catechol splitoff path was very smooth, the dehydrogenation featured an additional transition state in the form of an OH group rotation. The combined reaction was judged endothermic in the range of 0 K to 1250 K, and exergonic at 1000 K and above. It is shown that the catechol splitoff is the rate-determining step of the pyrolysis of catechin, which is equivalent to kinetic inhibition at all investigated temperatures.

CPP 35.34 Wed 11:00 P1

Pyrolysis of ellagic acid - a thermodynamic and kinetic study by means of quantum chemistry — •Philip Schöne, Jakob Kraus, and Jens Kortus — TU Bergakademie Freiberg (Institut für Theoretische Physik) Leipziger Str. 23, 09599 Freiberg, Deutschland

By performing ab-initio calculations, thermodynamic and kinetic data on the pyrolysis of ellagic acid were computed. The reaction path consists of two decarboxylations and two hydrolyses. The pyrolysis of ellagic acid can take place via the formation of either hexahydroxydiphenic acid or urolithin m5. Using select DFT functionals and quantum chemical methods, data for each reaction were calculated between 0 K and 1200 K. The occurring decarboxylations were found to be very similar to each other, being exothermic and exergonic reactions that become increasingly so with rising temperature. The hydrolyses show the opposite behavior, being slightly endothermic and endergonic reactions that become increasingly so with rising temperature. With the help of the climbing image nudged elastic band method, mechanisms for all reactions could be proposed and highest energy transition states could be identified. For the decarboxylations, these represent H transfers from the carboxylic group to the neighboring C atom. For the hydrolyses, the highest energy transition states correspond to H transfers from water to the nascent carboxylic group. Moreover, the rate-determining steps in the pyrolysis of ellagic acid were determined, which are the hydrolyses of urolithin m5 and luteic acid.

CPP 35.35 Wed 11:00 P1

Transversal piezo-force-microscopy with the use of interdigitated electrodes — •Maximilian Litterst, Andrey Butkevich, and Martijn Kemerink — Institute for molecular systems engineering and advanced materials, Heidelberg, Germany

Piezoresponse force microscopy (PFM) is a simple method to measure the piezoelectric effect of many materials with an atomic force microscope (AFM). Usually, a voltage is applied between the tip and the substrate to trigger a vertical displacement of the material via the converse, longitudinal, piezoelectric effect, which results in a vertical displacement of the tip. The transversal piezoelectricity can result in a torsion of the tip, it is however often very difficult to find a direct connection between the two.

Here, we present how interdigitated electrodes (IDEs) can be used to apply an electric field in the film-plane, resulting in a vertical displacement of the film due to the converse, transversal, piezoelectric effect. In addition, the longitudinal component can be measured via the torsional tip motion. This does not only provide a direct way to measure the transverse piezoelectricity, but also opens new possibilities for the device preparation.

CPP 35.36 Wed 11:00 P1

Ca substituion instead of Sr in $La_{0.58}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta}$ as a cathode electrode for IT-SOFCs — •Majid Jafari[1], Fatemeh Yadollahi Farsani[2], Norbert Menzler[3], Christian Lenser[4], and Fabian Grimm[5] — [1]Plön, Germany — [2]Isfahan university of technology, Isfahan, Iran — [3]Forschungszentrum Jülich, Jülich, Germany — [4]Forschungszentrum Jülich, Jülich, Germany — [5]Forschungszentrum Jülich, Jülich, Germany

$La_{0.58}Ca_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta}$ (L58CCF) was synthesized and evaluated as a cathode electrode for intermediate temperature solid oxide fuel cells (IT-SOFC) based on the Y_2O_3-stabilized ZrO_2 (YSZ) electrolyte. The effect of sintering temperature on the L58CCF performance was investigated. The best Area specific resistances (ASRs) for the L58CCF sintered at 950 °C were 1.218, 0.447, 0.228, 0.156, 0.099 $\Omega.cm^2$ at 600, 650, 700, 750, 800 °C, respectively.

CPP 35.37 Wed 11:00 P1

Antiperovskites ($(Li_2Fe)ChO$) as cathode material for lithium-ion batteries and investigation of the reaction mechanism — •Bowen Dong[1], Lennart Singer[1], Mohamed Abdullah Abdullah Mohamed[2], Silke Hampel[2], Nico Grässler[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Leibniz Institute for Solid State and Materials Research (IFW) Dresden e.V., Germany

Due to it unique structure, antiperovskite $(Li_2Fe)ChO$ (Ch = S, Se) have emerged as a promising Li-ion battery (LIB) cathode material with excellent rate capability and a good discharge capacity. We report synthesis of antiperovskites by a direct ball-milling process and evaluate the phase stability, cycling performance, and rate performance. The effect of post-synthesis heat treatment on the resulting materials as well as on its battery performance is studied. Cyclic voltammetry studies reveal a high-voltage decomposition process which progressively yields the formation of Fe_xCh_y. Galvanostatic measurements exhibit outstanding electrochemical cycling performance of antiperovskite-based cathodes of 250 mAh/g at 0.1 C. Further, we suggest a route to avoid the progressing conversion of $(Li_2Fe)ChO$ (Ch=S, Se) to Fe_xCh_y which effectively improves the cell performance of antiperovskites.

CPP 35.38 Wed 11:00 P1

Rational Design of Novel Photoswitches with Generative Models — •Robert Strothmann, Christian Kunkel, Johannes Margraf, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin, Germany

The sheer vastness of chemical spaces poses a daunting challenge to molecular discovery through high-throughput screening based on exhaustive sampling. Generative models (GMs) are an emerging machine learning (ML) approach that enables a more guided discovery. Implicitly learning chemical design rules from large reference data sets and suitable descriptors of a targeted functionality, GMs directly propose promising, yet diverse candidates.

Here we explore the use of GMs for the design of novel molecular photoswitches. In a first step, large general molecular databases are used to train a GM to generate chemically valid photoswitches. In a second step, the creation process needs to be conditioned towards performant switching capabilities. In the absence of sufficient corresponding experimental reference data, this conditioning is based on synthetic first-principles data. For that purpose computationally efficient descriptors are used in a multi-objective fashion to account for the desired key aspects of the switching process.

CPP 35.39 Wed 11:00 P1

Correlating molecular properties to nonlinear optical activity: Prerequisites for white light generation. — •Ferdinand Ziese, Lena Albohn, Kevin Eberheim, and Simone Sanna — Institut für Theoretische Physik Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Recent studies have demonstrated white light generation from molecular clusters with adamantane-like cores and different ligands [1,2]. To understand the origin of this behavior, we have investigated structural, electronic, and (nonlinear) optical properties from first principles for isolated molecules and dimer structures [3]. In this contribution, we focus on the comparison between isolated molecules and molecular dimers. We correlate the structural and electronic properties with the optical response and investigate the effect of symmetry and heterogeneous composition.

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CPP 35.40 Wed 11:00 P1

Effect of electron and laser irradiation on the structure of halogen substituted adamantane clusters — •Lena Albohn, Simone Sanna, Kevin Eberheim, and Ferdinand Ziese — Institu für Theoretische Physik Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Functionalized adamantane molecular clusters are highly nonlinear optical materials which are able to convert infrared radiation into a directed emission supercontinuum. While the origin of the optical nonlinearity is still under debate, the amorph habitus of the materials seems to be a prerequisite for the white-light generation.

Unfortunately, many adamantane-based or organotetrel clusters crystallize in an ordered structure characterized by intense second-harmonic generation instead of white-light emission. In order to render the molecular crystals amorph, electron or laser irradiation has been suggested. In order to explain the mechanisms leading to the structural modification, we model electron or laser irradiation from first principles. Thereby, we employ halogen substituted adamantane clusters as a model system. Our calculations reveal that laser and electron irradiation have a similar effect on the compounds. Depending on the irradiation dose, intermolecular rearrangements as well as intramolecular deformations (photochemical rearrangement) may occur, thus facilitating the white-light emission.

CPP 35.41 Wed 11:00 P1

Structural properties of a semi-dilute suspensions of magnetic multicore nanoparticles — •Ekaterina Novak[1], Andrey Kuznetsov[2], Elena Pyanzina[1], Marina Gupalo[1], Tatyna Belyaeva[1], and Sofia Kantorovich[2] — [1]Ekaterinburg, Russia — [2]University of Vienna, Vienna, Austria

During the last thirty years, magnetic soft matter systems have become highly promising candidates for medical applications such as magnetic hyperthermia and magnetic drug targeting. The subject of this work, magnetic multicore nanoparticles (MMNPs), are rigid clusters of single-domain magnetic nanocrystals (cores or grains) embedded in a polymer or other non-magnetic matrix. While the grains typically have a characteristic linear size of the order of 10 nm, the size of MMNPs can range from tens to a few hundred nanometers. Here, using Langevin dynamics computer simulations, we investigated diluted suspensions of MMNPs composed by grains, whose positions are fixed within the particle body, but their magnetic moments are free to rotate, corresponding to the grains with negligibly low magnetic anisotropy.

We calculated cluster size distributions and compared them to their counterparts in a system of single-domain magnetic nanoparticles. A drastic difference was found: for two MMNPs to aggregate they need to form a bridge a stable array of grains from both multicores that are connected via dipolar interactions. The more bridges the two MMNPs form, the more stable is their aggregate.

CPP 35.42 Wed 11:00 P1

Characterisation and transport within tetra-PEG*tetra-PCL amphiphilic end-linked polymer model networks — •Lucas Löser[1], Carolin Bunk[2], Frank Böhme[2], and Kay Saalwächter[1] — [1]Inst. F. Physik * NMR, Martin-Luther-Universität Halle-Wittenberg, Halle/D — [2]Leibnitz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, Dresden/D

A new approach for the synthesis of model-like amphiphilic co-networks is introduced, and their structure is analyzed by static 1H time-domain nuclear magnetic resonance (NMR) methods [1]. The hetero-complementary end-linking reaction of two well-defined star precursors [2] is implemented to obtain amphiphilic gels. We link PEG stars with hydrophobic poly-*-caprolactone stars (tetra-PCL), resulting in the formation of an amphiphilic network. NMR is shown to be capable of distinguishing different chain species in the swollen PEG-PCL networks, allowing quantification of network connectivity defects arising from the end-linking reaction, as well as accurate quantification of inelastic material. The mesh size of the networks is studied by Pulsed-Field Gradient (PFG) NMR, using dextrans as hydrophilic probe molecules for the network swollen in selective solvents. Furthermore, we performed measurements using small-angle x-ray scattering and 1H MAS recoupling NMR for information on the properties of the selectively swollen networks, e.g., estimates for the correlation length of PCL domains, and chem. shift-specific information about the chain dynamics. [1] Bunk et al.; Macromolecules 2022, 55, (15), 6573-6589 [2] Sakai, T. et al.; Macromolecules 2008, 41, (14), 5379-5384

CPP 35.43 Wed 11:00 P1

Hybrid hydrogel films for scalable H2 production — •Morgan Le Dû[1], Julija Reitenbach[1], Manuel A. Reus[1], Kun Sun[1], Zerui Li[1], Sigrid Bernstorff[2], Cristiane Henschel[3], André Laschwesky[3], Christine M. Papadakis[4], and Peter Müller-Buschbaum[1,5] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Elettra-Sincrotrone Trieste, Basovizza, Italy — [3]Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm, Germany — [4]TUM School of Natural Sciences, Soft Matter Physics group, Garching, Germany — [5]Heinz

Maier-Leibnitz-Zentrum (MLZ), TUM, Garching, Germany

The water splitting reaction can produce hydrogen-based energy from solar radiation. A promising photocatalyst for this reaction is Pt loaded graphitic carbon nitride (g-CN). It shows a high H2 evolution efficiency in aqueous solution. Previous works proposed to introduce hydrogels as host matrix and water storage to facilitate homogeneous spreading. This work aims to develop this system industrially scalable in a polymer thin film configuration. Poly(N-isopropylacrylamide) thin films exhibit good swelling capacity in water vapor atmosphere and appear suitable for a hybrid thin film system. A new isomer poly(N-vinylisobutyramide) seems also promising due to its higher lower critical solution temperature in aqueous solution. Therefore, a comparison of both polymers is based on in situ spectral reflectance and FT-IR measurements. The films have been spray coated to proceed grazing incident small angle x-ray scattering where g-CN/Pt blended polymer films microstructure was analysed under light irradiation.

CPP 35.44 Wed 11:00 P1

Effect of type of initiator and purification on the properties of thermo-responsive PNIPAM microgels — •Joanne Zimmer, Sebastian Stock, Souraj Mandal, Carina Schneider, Luca Mirau, and Regine von Klitzing — Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Germany

Microgels (MG) are polymeric networks in the size range of micrometers boasting properties of both colloids and polymers. Depending on their composition MG can respond to external stimuli such as temperature or pH. An example of a thermo-responsive polymer is Poly(N-isopropylacrylamide) (PNIPAM). PNIPAM MG can be synthesized by surfactant-free precipitation polymerization comprising NIPAM monomers, the crosslinker N,N'-methylenebisacrylamide (BIS) and a radical initiator. Depending on the radical initiator, either negatively or positively charged MG are generated. The subject of this work is the evaluation of the MG charge on the thermo-responsive swelling behavior and elastic properties using Dynamic Light Scattering and Atomic Force Microscopy. In addition, the type of MG purification and its effect on the resulting MG properties is investigated. It was shown, that the presence of undesired low-molecular weight products strongly impacts the MG interfacial adsorption behavior what we wish to understand. In this regard, sufficient removal was only achieved if, apart from the standard purification via dialysis, subsequent centrifugation steps were carried-out. The MG bulk properties (hydrodynamic radius, Zeta-potential) remained unchanged before and after centrifugation.

CPP 35.45 Wed 11:00 P1

Diketopyrrolopyrroles on graphite: Carpets self-assembled via hydrogen bonding — Moufdi Hadjab[1,2], Vladyslav Savchenko[2], Nina Tverdokhleb[2], and •Olga Guskova[2] — [1]Mohamed Boudiaf University of M'sila, Algeria — [2]IPF Dresden, Germany

We investigate the initial stages of the adsorption and thin-film formation of N-unsubstituted difuryl-diketopyrrolopyrroles (DPP) on graphite. Molecules in a particular conformational state (cis-cis, cis-trans or trans-trans) build the adsorption layers during in-silico self-assembly on surface through intermolecular hydrogen bonding. Here, the vacuum deposition of the molecules is reproduced in the all-atom MD setup [1]. We found out the formation of stable carpets made of molecular stripes. These carpets can be characterized as monomolecular layers in contrast to the sructures, formed using droplet deposition [2]. The most stable stripes are made of cis-cis conformers, which is explained by stronger intermolecular hydrogen bonding. The stripe growth is accompanied by the reduction of the Eg gap. At the same time, the binding energy of the molecules does not show a clear dependence on the stripe length, which is a signature of the isodesmic self-assembly. Additionally, we quantify the intermolecular and the molecule/graphite energies for the hydrogen-bonded DPP molecules and compare the results with known experimental data. This work is supported by DFG, grant GU1510/5-1. [1] Guskova O.A., et al. J. Phys. Chem. C 2013, 117, 33, 17285. [2] Hadjab M., Guskova O. Herald of TvSU. Ser. Chem. 2021, 4, 46, 118.

CPP 35.46 Wed 11:00 P1

Ground- and excited-state properties of tetraphenyl compounds from first-principles calculations — •Kevin Eberheim, Lena Albohn, Ferdinand Ziese, Christof Dues, and Simone Sanna — Institut für Theoretische Physik and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

Tetraphenyl compounds with formula $X(C_6H_5)_4$ (X being a tetravalent atom of the 14th group such as C, Si, Ge, Sn, Pb), crystallize either in a tetragonal crystalline structure or in an amorph phase [1]. Depending on their habitus, the compounds are characterized by very different optical properties. The molecular crystals are known for their second harmonic generation (SHG) properties, while the amorph phase is a white light emitter. Tetraphenyl molecules feature indeed the delocalized π-orbitals, which have been proposed as a prerequisite for the white-light generation [2]. In an attempt to understand the mechanisms related to the white light emission, we model the structural, electronic and vibrational properties of different $X(C_6H_5)_4$ structures within density functional theory. The calculated structural parameters closely reproduce the measured values, however vdW corrections are crucial for a correct description of the structural properties. This con- firms that dispersion forces are responsible for the intermolecular bonds in the compound. Different implementations of the vdW forces lead to very similar results. Calculated vibrational properties are in agree- ment with measured Raman spectra. [1] A Kitaigorodsky, Molecular crystals and Molecules, Acad. Press (1973). [2] Nils W. Rosemann et al., J. Am. Chem. Soc. 138, 16224 (2016), Science 352, 1301 (2016).

CPP 35.47 Wed 11:00 P1

Scaling Properties of Tree-like Self-Similar Polymers — •Ron Dockhorn[1] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institut für Theoretische Physik, D-01069 Dresden, Germany

In this study, regular polymeric Vicsek- and T-fractals are compared to dendrimers in means of theory and simulations. Albeit all structures exhibit exponential growth both for the number of monomers inside the structures and also for the terminal groups their structural properties differ significantly. Computer simulations are performed to investigate the scaling properties of the tree-like self-similar polymers utilizing the Bond-Fluctuation-Model with the Metropolis method as well as with the Wang-Landau algorithm. The radius of gyration, the heat capacity and the θ-point of those systems is investigated to examine the coil-globule transition of the polymeric fractals. A mean field theory for the scaling exponent in different solvent regimes is applied and found in fair agreement to the simulation data. A cross-over from almost linear chain behavior to spherical shape is observed, which can be tuned by the intrinsic functionality of the building blocks. The polymeric fractals can be an alternative to dendrimers in the class of hyperbranched polymers.

CPP 35.48 Wed 11:00 P1

Statistical Analysis of the Dimerization of Polyglutamine Chains — •Christian Lauer and Wolfgang Paul — Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

We are presenting a numerical investigation of the dimerization of polyglutamine homo-peptides of varying length. We use the intermediate resolution protein model PRIME20 and study it with a flat-histogram type Monte Carlo simulation. This gives us access to the thermodynamic equilibrium of this model over the complete control parameter range, which for our simulations is the temperature. For densities comparable to typical in vitro experimental conditions we find that the aggregation and folding of the polyglutamine chains occur concurrently. However, as a function of chain length the sequence of establishment of intra- and intermolecular hydrogen bonding contacts changes. Chains longer than about $N = 24$ polyglutamine repeat units fold first and then aggregate. This agrees well with the experimental finding, that beyond $N = 24$ the single polyglutamine chain is the critical nucleus for the aggregation of amyloid fibrils. A finite size scaling of the ordering temperatures reveals that for this chain length (and longer chains) folding occurs at physiological (respectively larger) temperatures whereas shorter chains are disordered at physiological conditions.

CPP 35.49 Wed 11:00 P1

Construction of a polarizable force field for molecular dynamics simulation of a NaOTF Water-in-Salt electrolyte — •Majid Rezaei, Sung Sakong, and Axel Gross — Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany

A NaOTF Water-in-Salt (WiS) electrolyte is modeled using classical molecular dynamics (MD) simulations. For this, four different force fields are employed to account for atomic polarization at different levels: a non-polarizable all-atom force field where the polarization effect is only implicitly included in the Van der Waals interaction parameters; the same force field with uniformly scaled ionic charges which, in a mean-field approximation, mimics electron polarization; a partially polarizable force field where ion polarization is explicitly accounted for via Drude oscillators while water is modeled by the non-polarizable SPC/E model; and a fully polarizable force field where the Drude oscillator model is used to account for both water and ion polarization. The primary goal of this study is to evaluate the simulation stability when using the above force fields and to investigate how the electrolyte properties are sensitive to the force field parameters. The results are then used to construct a force field that best reproduces the electrolyte properties obtained from ab initio molecular dynamics (AIMD) calculations. For this purpose, we use the partially polarizable model, which we believe is accurate enough to reproduce various properties of the studied electrolyte while the computational effort is affordable. The optimized force field will then be used to study the structure and dynamic properties of a NaOTF WiS solution under different conditions.

CPP 35.50 Wed 11:00 P1

Kirkwood-Buff theory approach towards cosolvent effects on single polymer chain collapse transition — •Martin Melčák, Jakub Smutek, and Jan Heyda — Department of Physical Chemistry, University of Chemistry and Technology, Prague, Technická 5, CZ-16628 Praha 6, Czech Republic

The so-called smart materials are unique for their ability to rapidly and fully reversibly change physical or chemical properties upon exposure to external stimuli, such as temperature, light, pH, or solvent quality. In this contribution, we have taken under focus the prominent example of thermoresponsive polymer, which conformation can be near critical temperature modulated by the addition of small doses of cosolvents. To reveal the microscopic origin of the thermodynamic effect, we employed coarse-grained molecular dynamics simulations of a single polymer chain in mixed solution. The studied model can effectively describe changes in polymer chain conformation as well as the responses of the local solution composition in polymer proximity. Utilizing this fact, we have described and analyzed system thermodynamics in the framework of Kirkwood-Buff theory, which combines the polymer and environmental perspective of cosolvent effect on the polymer transition. Within a single unifying concept, our model is thus capable to quantitatively describe cosolvent effects in three interaction regimes, namely: depleted, weakly binding, and bridging regime.

CPP 35.51 Wed 11:00 P1

Fabrication of Plasmonic Au Nanostructures for Electrocatalysis — •Gina Ross and Björn Braunschweig — Institut für Physikalische Chemie, WWU Münster, 48149 Münster, Germany

Nanosphere lithography (NSL) is a classical technique to fabricate reproducible 2D masks. These masks can be used to structure surfaces in a well-defined fashion. We have used spherical polystyrene (PS) particles to generate closed-packed hexagonal layers on a substrate surface that serves as a quasi 2D mask. The latter is subsequently coated with Au to fabricate Au nanopyramids which are received by dissolution of the PS particles. Their deposition as a mask was done with the Langmuir-Blodgett transfer at the air-water interface. For that a suspension of polystyrene particles was spread on the water subphase containing no additional salt or surfactant. The fraction of PS particles sinking into the bulk subphase was drastically reduced by a 1:1 suspension of water and ethanol, and by dispensing the PS suspension onto the air-water interface with a glass slide at an angle of 45° relative to the interface. Au deposition and mask removal with an ultrasonic bath led to the formation of Au nanopyramids. We expect the interaction of these nanostructures with electromagnetic radiation to result in a local field enhancement which promises to improve chemical reactions sensitive to electric field gradients. For that reason we have investigated the ability of Au plasmonic structures to promote CO_2 electrocatalysis.

CPP 35.52 Wed 11:00 P1

Luminescence properties of Nd complexes and processing of photonic crystal structures — •Miriam Gerstel[1], Ingo Köhne[2], Paul Mertin[3], Bernd Witzigmann[3], Johann Peter Reithmaier[1], Rudolf Pietschnig[2], and Mohamed Benyoucef[1] — [1]Institute of Nanostructure Technologies and Analytics — [2]Institute of Chemistry, CINSaT, University of Kassel, Germany — [3]EEI Department, Friedrich-Alexander University of Erlangen-Nürnberg, Germany

Lanthanide ion luminescence exhibits characteristic narrow emission bands along with relatively long emission lifetimes which makes them attractive for applications in lighting, sensing, and display technologies. We investigate the optical characteristics of phosphonate ester-supported nitrite and chloride neodymium(III) complexes as solid bulk material and in solution. Optical properties of Nd complexes are determined by photoluminescence (PL) spectroscopy, which reveals emission bands of Nd(III) ions in the NIR region. PL measurements of equimolar solutions reveal information about the emission strength of the complexes with different ligand types. Temperature-dependent PL spectra enable the assignment of the emission lines observed around 880 nm. For light enhancement, molecules are immobilized on photonic crystal cavities (PhCs). The fabrication of PhCs by electron-beam lithography, inductively coupled plasma reactive ion etching and selective wet etching techniques is discussed. This work is supported by the state of Hesse in the frame of LOEWE priority project SMolBits and the DFG grant-BE 5778/4-1.

CPP 35.53 Wed 11:00 P1

Insights into structure and dynamics of polycaprolactone-based star-shaped polymer electrolytes from molecular dynamics simulations — •Mirko Fischer[1], Diddo Diddens[2], and Andreas Heuer[1] — [1]Institute of Physical Chemistry, Westfälische Wilhelms-Universität Münster, Münster 48149, Germany — [2]Forschungszentrum Jülich GmbH, Helmholtz Institute Münster, Münster 48149, Germany

Solid polymer electrolytes (SPEs) are promising candidates to substitute classical organic electrolytes in lithium-ion batteries, as they are chemically and mechanically more stable and have improved safety. However, they exhibit low ionic conductivity, which can be generally improved by developing novel polymer architectures. Experiments have shown that the biodegradable Grafted Cyclodextrin-Polycaprolactone (GCD-PCL) has higher transfer numbers than classical poly(ethylene oxide). In this work, we present results of molecular dynamics (MD) simulations to understand the ion transport in GCD-PCL. In order to directly compare our simulations with experiments, we used the time-temperature superposition of mean residence times and mean squared displacements of lithium ions to calculate the ionic conductivity at low temperatures, which would otherwise require larger time scales than are accessible through MD simulations.

CPP 35.54 Wed 11:00 P1

Organisation of Nanoparticles with Polymer Brushes: Computer Simulation Studies — •Bhuwan Poudel, Hsiao-Ping Hsu, and Kurt Kremer — Max Planck Institute for Polymer Research, Mainz, Germany

For polymer brushes containing nanaoparticles, the interplay between concentration of nanoparticles and interaction between monomers and nanoparticles affects the ordering of nanoparticles and the structural and dynamical properties of the respective polymer brushes. We perform molecular dynamics simulations of polymer brushes based on the bead-spring model and treat nanoparticles as hard spheres with a diameter six times larger than the monomer size. Initially, nanoparticles are randomly distributed inside or above the polymer brushes. By tuning the attractive interaction between monomers and nanoparticles, we study the assembly of nanoparticles within the polymer brushes as a function of nanoparticle concentration. The appropriate choice of monomer-nanoparticle interaction and concentration of nanoparticles gives rise to a single (ordered) layers of nanoparticles whose equilibrium positions fluctuate within their diameters.

CPP 35.55 Wed 11:00 P1

Tribological Properties of Selected Vanadium Oxides Investigated with *ReaxFF* molecular dynamics — •Miljan Dašić[1,2], Ilia Ponomarev[1], Tomaš Polcar[1], and Paolo Nicolini[1] — [1]Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, Technicka 2, Prague 6, 16627, Czech Republic — [2]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

Providing effective lubrication at high temperatures/pressures and in oxidative environments is relevant for various industrial applications, such as turbomachinery and cutting tools. Promising solutions are oxidation-resistant hard coatings consisting of binary or ternary films (e.g., $Cr-N$, $Ti-N$, $Cr-Al-N$, $Ti-Al-N$) doped with vanadium. The amount of oxygen present in an oxidative environment can be varied, leading to different vanadium oxide stoichiometries. We investigated tribological performance of under-oxidized vanadium lubricants, selected based on available experiments. We conducted a *ReaxFF* molecular dynamics study on selected stoichiometries {V_2O_3, V_3O_5, V_8O_{15}, V_9O_{17}, VO_2} at elevated temperatures {600, 800, 1000} [K] and pressures {1, 2, 3, 4} [GPa]. Our tribosystem consists of two rigid V_2O_5 layers, and a vanadium oxide in-between. At a fixed temperature, we did not notice significant changes of the friction coefficient with stoichiometry. All considered stoichiometries provide effective lubrication. Our study is relevant and interesting for the design of vanadium doped oxidation-resistant hard coatings.

CPP 35.56 Wed 11:00 P1

interfacial rheology of PNIPAM aqueous solutions at air-water interface: effect of cross-linking and oscillation frequency — •Atieh Razavi, Regine von Klitzing, and Amin Rahimzadeh — Hochschulstraße 8, 64289 Darmstadt, Germany

PNIPAM microgels are swollen and dispersible in water at temperatures below their VPTT .Microgels tend to adsorb at the liquid-air interface, thus reducing the surface tension. The degree of crosslinking influences the required time to reach the steady state. Higher cross-linker content results in a longer transient time in the order of several minutes (depending on the solution concentration). Upon the formation of a new interface, this transient time together with the mechanical properties of microgels play key roles in the interfacial elasticity of the air-water interface. The dynamic surface elasticity of aqueous solutions of PNIPAM has been measured by the oscillating barrier method as a function of time and concentration in different surface elongation frequencies. Results shows the apparent dilational elastic and loss moduli deduced from the pendant drop shape analysis at the air*water interface, as a function of pressure for the three cross-linking densities: 1, 5 and 10 mol%. In all cases, the apparent elastic modulus is much larger than the apparent loss modulus. The magnitude of the different elastic moduli goes through a maximum of elasticity for pressure values of about 15 mN/m. This behavior is a direct consequence of the particular structure of microgels, i.e. a dense and rigid core surrounded by a deformable shell made of dangling chains.The effect of oscillation frequency is still challenging and open question.

CPP 35.57 Wed 11:00 P1

Diffusion controlled pairwise associations of telechelic polymer chains — •Michael Lang and Ron Dockhorn — Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, Hohe Straße 6, 01069 Dresden, Germany

We study the pairwise association of telechelic chains in polymer melts. We derive the life time distributions of open stickers that return to the same partner as before (return walks) and the life time distribution of open stickers that exchange their binding partners (exchange walks) for both entangled and non-entangled chains. These distributions contain the full information of the bond association dynamics and allow to develop a generalization of the law of mass action in the diffusion controlled limit. The model predictions are tested by Monte-Carlo simulations and compared with preceding work on associations in networks.

CPP 35.58 Wed 11:00 P1

Architecture effect on the behavior of gradient and triblock terpolymer OEGMA-BuMA-DEGMA — •Wenqi Xu[1], Eirini Melampianaki[1], Feifei Zheng[1], Anna P. Constantinou[2], Theoni K. Georgiou[2], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Department of Materials, Imperial College, London, England

Triblock terpolymers with hydrophilic, hydrophobic, and thermoresponsive blocks feature micellization, aggregation, and gelation in response to temperature changes and are therefore promising in various biomedical applications [1]. Gradient terpolymers can serve as a cost-effective alternative. Here, we investigate a triblock and a gradient terpolymer composed of hydrophilic oligo(ethylene glycol) methyl ether methacrylate (OEGMA), hydrophobic *n*-butyl methacrylate (BuMA), and thermoresponsive di(ethylene glycol) methyl ether methacrylate (DEGMA). Dynamic light scattering and synchrotron small-angle X-ray scattering revealed that the gradient terpolymer forms spherical micelles, whereas the triblock terpolymer is apt to form elongated micelles. With increasing temperature, the former grow in radius and the latter in length, which may be due to the increasing hydrophobicity of the DEGMA block.

[1] A. P. Constantinou, L. Wang, S. Wang, T. K. Georgiou, Polym. Chem. 2022., doi: 10.1039/D2PY01097F

CPP 35.59 Wed 11:00 P1

Adaptive Air-Water Interfaces with Spiropyran and Arylazopyrazole Photoswitches — •Michael Hardt and Björn Braunschweig — University Münster, Center for Soft Nanoscience, 48149 Münster, Germany

Interfaces that respond to stimuli such as light or temperature are of great interest for new intelligent materials. Using molecular switches that respond to orthogonal triggers, the properties of fluid interfaces can be preconditioned and a low level of adaptivity can be integrated that extents the possibilities of soft matter interfaces beyond responsive functions.

In this contribution, we report on the adaptive behavior of air-water interfaces that are decorated by spiropyran (SP) and arylazopyrazole (AAP) photo-responsive surfactants. The SP surfactants increase their surface activity when irradiated with UV light that causes a ring-closure reaction. E/Z photo-isomerization of the AAP surfactants drives a substantial decrease in surface activity and thus desorption from the interface when the AAP surfactants are switched from their E to the Z state. In addition, at low pH the short thermal lifetime of the Z state as well as of the SP form offers the use of thermal relaxation as an alternative trigger, while also irradiation with green light can partially recover the initial properties. Interfacial properties and molecular kinetics were studied in detail using surface tensiometry and vibrational sum-frequency generation (SFG).

CPP 35.60 Wed 11:00 P1

A thermo- and photoresponsive polymer for schizophrenic switching of amphiphilic self-assembled micelles — •Peiran Zhang[1], René Steinbrecher[2], André Laschewsky[2,3], Peter Müller-Buschbaum[4], and Christine M. Papadakis[1] — [1]Soft Matter Physics Group, TUM School of Natural Sciences, Technical University of Munich — [2]Institute of Chemistry, University of Potsdam — [3]Fraunhofer IAP, Potsdam-Golm — [4]Chair for Functional Materials, TUM School of Natural Sciences, Technical University of Munich

Schizophrenic switching, namely the exchanging of hydrophilic and hydrophobic segment of an amphiphilic diblock copolymer, leads to self-assembly of micelles and inverse micelles, which can be used in the drug delivery application [1]. We aim to achieve such behavior by means of diblock copolymers composed of a thermo-responsive block with a fixed LCST (lower critical solution temperature) and a photo-responsive block with a tunable LCST, which is accomplished by cis-trans isomerization of the incorporated azobenzene group. As a first step, we use turbidimetry and dynamic light scattering (DLS) to investigate a homopolymer precursor with respect to the cloud point and the chain size in the cis- and trans-form of the azobenzene group, which is realized by 365 nm UV light and 470 nm blue light, respectively.

[1] C. M. Papadakis, P. Müller-Buschbaum, A. Laschewsky, Langmuir 2019, 35, 9660-9676.

CPP 35.61 Wed 11:00 P1

Effect of pressure on the micellar structure of PMMA-*b*-PNIPAM in aqueous solution — •Pablo A. Alvarez Herrera[1], Geethu P. Meledam[1], Cristiane Henschel[2], Leonardo Chiappisi[3], André Laschewsky[2], and Christine M. Papadakis[1] — [1]TU München, School of Natural Sciences, Garching Germany — [2]Universität Potsdam, Institut für Chemie, Potsdam-Golm, Germany — [3]Institut Laue- Langevin, Grenoble, France

In aqueous solution, amphiphilic diblock copolymers consisting of a permanently hydrophobic and a thermo-responsive block self-assemble into core-shell micelles. In particular, poly(methyl methacrylate)-*b*-poly(*N*-isopropylacrylamide) (PMMA-*b*-PNIPAM) forms micelles featuring a hydrophobic PMMA core and a thermo-responsive PNIPAM shell. This phase transition can be also induced by changing the pressure. Here, we study the effect of pressure on the micellar structure of PMMA-*b*-PNIPAM in aqueous solution by small-angle neutron scattering (SANS). In temperature-resolved experiments, we find that the micellar shell strongly dehydrates after crossing the co-existence line at 0.1 MPa. At 75 MPa, on the contrary, it remains hydrated and the micelles are highly-correlated within the aggregates. We also characterized the micellar structure in a pressure-resolved experiment at 31.8 °C. In this case, we find that, after crossing the co-existence line, the micellar shell appreciably shrinks, even though it remains partially hydrated. We conclude that the micellar structure in the two-phase region strongly depends on pressure.

CPP 35.62 Wed 11:00 P1

Synthesis of diblock copolymer brush surfaces to control the adaptation time to water — •Benjamin Leibauer[1], Andres de los Santos Pereira[2], Ognen Pop-Georgievski[2], Hans-Jürgen Butt[1], and Rüdiger Berger[1] — [1]Max-Planck institute for polymer research, Ackermannweg 10, 55128 Mainz — [2]Institute of macromolecular chemistry cas, Heyrovskeho nam. 1888, 162 00, Praha 6

The Young's model describes the wetting behavior of an ideal surface. Recently, Butt et al. presented a model, which connects adaptation processes of the surface to dynamic contact angles. We developed an experimental setup, which allows measuring adaptation processes. The adaptation model was experimentally verified by Li et al. using surfaces coated with films of statistical copolymers. We synthesize polymer brush surfaces with the aim to control the adaptation time scale upon wetting and dewetting systematically. We used the surface-initiated atom transfer radical polymerization / ATRP to selectively synthesize diblock copolymer brushes. We prepared poly(2-hydroxyethyl methacrylate) (PHEMA) as a hydrophilic block from the surface and we grafted polystyrene (PS)) as hydrophobic block on top of the PHEMA block. By regulating the architecture and thickness of the polymer brush we can tune surface adaption to wetting.

CPP 35.63 Wed 11:00 P1

Droplets sliding on compressed soft surfaces — •Youchuang Chao, Hansol Jeon, and Stefan Karpitschka — Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany

The motion of droplets on rigid substrates is mainly slowed up by the viscous dissipation inside the liquid phase. However, this does not hold for droplets sliding on soft substrates: viscoelastic dissipation inside solid phase now dominates the motion, leading to 'viscoelastic breaking". A recent study revealed that droplets move anisotropically on soft, pre-stretched solids, which is incompatible with the classical visco-elastocapillary wetting theory. Here, we impose a compression rather than a stretch on the soft solid, and explore how pre-compression influences the droplet speed. Intriguingly, we observe a non-monotonic dependence of the sliding speed on the pre-strain: a minimal speed exists as the solid is consecutively compressed. This may enrich our current understanding of elastocapillarity, for instance, in tissue engineering where soft materials are frequently squeezed.

CPP 35.64 Wed 11:00 P1

Understanding wetting and drying of nanoporous media through optical and dilatometry experiments — •Laura Gallardo[1,2,3], Juan Sánchez[1,2,3], Yannick Tetzner[1,2,3], and Patrick Huber[1,2,3] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Photon Sciences, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [3]Center for Hybrid Nanostructures CHyN, Hamburg University

While imbibition kinetics is well-understood in nanoporous materials [1], their drying dynamics is still under investigation [2]. In this study, we present time-dependent macroscopic dilatometry experiments on the deformation of nanoporous monoliths upon spontaneous, capillarity-driven infiltration of water as well as drying. During both processes, we find characteristic dynamical regimes that can be quantitatively described in terms of Laplace pressure effects and changes in the surface stress at the inner pore walls [3]. In the particular case of transparent nanoporous Vycor glass, additional imaging experiments are conducted, allowing direct optical access to the filling front. The observed wetting-drying dynamics are consistent with our analysis of the strain regimes. Our study demonstrates that it is possible to monitor the interplay of imbibition and drying dynamics by simple dilatometry measurements, provided proper humidity control. [1] Gruener, et al (2009), Phys. Rev. E Stat. Nonlin. Soft Matter Phys., 79(6). [2] Al-Madani, R. (2018), Conference paper: YUCOMAT2018. [3] Gor, G. Y., et al. (2017). Appl. Phys. Rev., 4(1), 011303

CPP 35.65 Wed 11:00 P1

Studying Solid-liquid Contact Charge Separation Dynamics using Mirror Charge — •Pravash Bista[1], Hans-Jürgen Butt[1], and Stefan A.L Weber[1,2] — [1]Max-Planck-Institut for Polymer research Mainz — [2]Johannes Gutenberg University of Mainz

Charge separation as water drops slide over a hydrophobic solid surface is a well known phenomenon (Slide electrification). Nevertheless, a macroscopic understanding of dynamics in solid-liquid contact charge separation is still incomplete. To address that, we introduce a method based on "*mirror charge*" detection to locally measure the change in surface charge density ($\Delta\sigma$). Here, we placed a grounded metal electrode parallel beneath the substrate. As a spontaneously charged drops move over a surface, they attract opposite charge in the metal electrode causing a flow of capacitive current. Analysing this current, we studied $\Delta\sigma$ dynamics with increasing slide length and drop number as multiple deionized water drops slid down the inclined hydrophobic surface (trichloro(1H,1H,2H,2H-perfluorooctyl)silane, PFOTS-functionalized glass). Using the results, we estimated a set of parameters to describe the $\Delta\sigma$ dynamics in slide electrification. Further, we used these parameters in a numerical simulation where we numerically reproduced the experimental results.

CPP 35.66 Wed 11:00 P1

Towards wetting on switchable and adaptive conducting polymer surfaces — •Junqi Lu[1], Aldilene Santos Franca[1], Nikolaos Karadimitriou[2], Holger Steeb[2], and Sabine Ludwigs[1] — [1]IPOC-Functional Polymers, Institute of Polymer Chemistry, University of Stuttgart, Germany — [2]Institute of Mechanics (MIB) & SC SimTech, University of Stuttgart, Germany

Conducting polymers (CPs) are discussed in a huge variety of electronic devices including electrochromic windows, batteries, actuators and chemical-biology sensors, mainly because of switchable electronic and optical properties. Compared to other conducting materials, CPs have advantages of light-weight, low cost, non-toxicity, flexibility, easy processing, and low voltage operation. In our group, poly(3-hexylthiophene) (P3HT) and poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) are mostly studied. In the case of P3HT, the doping states can be precisely controlled by electrochemical or chemical doping, which results e.g. in an increase of conductivity over 6 orders of magnitude with a maximum of 224 S/cm. [1] On the other hand, PEDOT: PSS can be controlled by electrochemical means, but also by humidity, as used e.g. for actuators. [2] In this contribution, we will show our preliminary data on the wetting behavior on such switchable and adaptive CP surfaces.

Ref.: [1] Chem. Mater. 2020, 32, 14, 6003; [2] Adv. Mater. 2021,33, 2007982

CPP 36: Organic Electronics and Photovoltaics II (joint session CPP/HL)

Time: Wednesday 15:00–17:30 Location: GÖR 226

CPP 36.1 Wed 15:00 GÖR 226

Charge-carrier dynamics across seven orders of magnitude in double-cable polymer-based single-component organic solar cells — •Yakun He[1,2], Bingzhe Wang[1], Larry Lueer[1], Dirk Guldi[1], Ning Li[1], and Christoph Brabec[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Martensstrasse 7, 91058 Erlangen, Germany — [2]KAUST Solar Center, King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia

Single-component organic solar cells (SCOSCs) with intrinsically high stability have witnessed efficiencies from 2-3% to 6-11%. For boosting higher efficiencies of SCOSCs, essential information of charge-carrier dynamics as a function of microstructure is highly demanded, requesting systematical investigation on photophysics. In this work, for the first time, the charge-carrier dynamics of a representative double-cable polymer, which achieves efficiencies of over 6% as an active layer in SCOSCs, is investigated across seven orders of magnitude in time scale, from fs-ps TAS and ps-ns TRPL for probing charge generation to ns-us TAS for charge recombination. Specific emphasis is placed on understanding the impact of thermal post-treatment on the charge dissociation, transport, and recombination dynamics. By increasing the thermal annealing temperature, geminate recombination is reduced accompanied by more efficient charge dissociation and suppressed bimolecular recombination. Annealing the photoactive layer at 230 oC results in the highest photovoltaic performance correlating well with the findings from transient studies. This work intends to present a complete picture of the charge-carrier dynamics in SCOSCs.

CPP 36.2 Wed 15:15 GÖR 226

What determines the Recombination Order in Organic Solar Cells? — •Kathrin Brocker, Jana Seiler, Dorothea Scheunemann, Clemens Göhler, and Martijn Kemerink — Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University

Organic Solar Cells provide an interesting and low-cost alternative to conventional inorganic photovoltaics. Upon illumination, excitons are created that separate into free electrons and holes at the donor-acceptor-interface and can be extracted to deliver electricity. The opposing loss mechanism is the recombination of charge carriers, which happens in the bulk both prior to and after charge separation. To understand these processes, the recombination order is crucially important. Experimentally, orders around or above 2 are typically found. Surprisingly, kinetic Monte Carlo (kMC) simulations that otherwise accurately reproduce experimental observations, yield values closer to 1. Here, we investigate the factors that might lead to higher recombination orders. Apart from the influence of morphology and contacts, special focus is laid on the effect of charge carrier delocalisation, which is shown to facilitate charge carrier separation and increase the fraction of bimolecular recombination. Simulation results are compared to experimental data obtained via the Steady State Bias Assisted Charge Extraction (BACE) method on P3HT:PCBM and PM6:Y6 solar cells.

CPP 36.3 Wed 15:30 GÖR 226

Modeling of the photoluminescence of geminate pairs using a hopping based Monte Carlo simulation — •Maik Schwuchow, Angela Thränhardt, Carsten Deibel, and Sibylle Gemming — TU Chemnitz, Institut für Physik, 09126 Chemnitz, Deutschland

The investigation of the transport and recombination characteristics of optically excited charge carriers in organic materials is an on-going research topic. Studying the underlying effects is crucial for understanding and improving practical applications, e.g. organic solar cells (OSCs). A main step in the process of free charge carrier generation in OSCs is the formation of geminate pairs, so called charge transfer complexes, consisting of spatially separated, Coulomb-bound charges. The radiative recombination of geminate pairs yields a photoluminescence (PL) decay $\propto t^{-3/2}$ (t is time) on long time scales which arises due to a combination of thermally activated diffusion and attractive Coulomb interaction. While a continuous drift-diffusion model is able to theoretically explain this experimentally observed decay, weak molecular interaction and disorder are known to cause charge carrier localization. Therefore, a hopping model, based on tunneling between localized states, is usually more appropriate to describe charge transport in organic materials. We simulate the diffusion and recombination of hopping charge carriers using the Monte Carlo method and investigate the influence of different parameters, e.g. temperature and energetic disorder, on the PL data and the asymptotic slope.

CPP 36.4 Wed 15:45 GÖR 226

Time-consistent hopping, transient localization, and polarons - new insights and approaches for carrier transport in organic crystals — Sebastian Hutsch, Michel Panhans, and •Frank Ortmann — Technische Universität München, Germany

Charge transport in organic semiconductors is affected by the complex interplay of electronic degrees of freedom and molecular vibrations. This is further complicated due to the rich vibrational spectrum of these materials with mode energies covering two orders of magnitude. If the electronic coupling between molecules is small, hopping approaches are a popular choice to model charge transport for which we have recently derived a time-consistent hopping theory. [1]

Similarly, for high-mobility materials a recent improvement has been realized based on a mode-specific treatment of molecular vibrations. This leads to an unprecedented level of accuracy for the prediction of the carrier mobility for a large number of systems. [2] I will finally discuss physically motivated predictors with a very good correlation to the mobility and low computational costs.

[1] S. Hutsch, M. Panhans and F. Ortmann, Phys. Rev. B. 104, 054306 (2021).

[2] S. Hutsch, M. Panhans and F. Ortmann, npj Comput. Mater. 8, 228 (2022).

CPP 36.5 Wed 16:00 GÖR 226

Analysis of industrial viability for single-component organic solar cells — •Yakun He[1,2], Ning Li[1], Thomas Heumüller[1], Jonas Wortmann[1], and Christoph Brabec[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Martensstrasse 7, 91058 Erlangen, Germany — [2]KAUST Solar Center, King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia

Despite approaching 20% efficiency, organic solar cells still lag behind for industrial application. The industrial figure of merit (i-FOM) of OSCs is analyzed, including PCE, photostability, and synthetic complexity (SC) index. Single-component organic solar cells (SCOSCs) employing materials with donor and acceptor moieties chemically bonded within one molecule or polymer exhibit intrinsically high morphological stability. SCOSCs exhibit overall much higher i-FOM values than the corresponding bulk heterojunction OSCs, and the highest value reaches 0.3, which is even higher than the famous PM6:Y6, even though the PCE (8%) is only half of PM6:Y6. Synthetic complexity of SCOSCs is slightly higher than that of the corresponding BHJ OSCs due to extra synthetic step for connecting donor and acceptor moieties. This feature however overcomes the large-scale phase separation and stability issue. SCOSCs based on dyad 1 exhibit surprisingly high photostability under concentrated light (7.5 suns and 30 suns), corresponding to almost unchanged device stability up to 10,000 hours under 1-sun illumination. For realizing industrial application, SCOSCs have to achieve higher efficiencies, while BHJ should be developed with less complicated synthesis.

15 min. break

CPP 36.6 Wed 16:30 GÖR 226

Temperature-induced morphology changes at the organic-metal interface: effects on the structure, electronic and thermoelectric performance — •Benedikt Sochor[1], Yusuf Bulut[1,2], Marie Betker[1,3], Anna Lena Oechsle[2], Simon Schraad[1,4], Christopher R. Everett[2], Constantin Harder[1,2], Tzu-Yen Huang[5,6], Anton Le Brun[5], Tim Laarmann[1,4], Peter Müller-Buschbaum[2,7], and Stephan V. Roth[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, James-Franck-Str. 1, 85748 Garching, Germany — [3]KTH Royal Institute of Technology, Teknikringen 56-58, 100 44 Stockholm, Sweden — [4]University Hamburg, Department of Physics, Notkestr. 85, 22607 Hamburg, Germany — [5]ANSTO, New Illawarra Road, Lucas Heights, NSW 2234, Australia — [6]NSRRC, 101 Hsin-Ann Road, Hsinchu Science Park, Hsinchu 30076, Taiwan — [7]MLZ, TUM, Lichtenbergstr. 1, 85748 Garching, Germany

Flexible organic electronics are one of the most sought-after devices in the field of photovoltaics, sensors, or smart wearables. Here, the structure of the organic-metal interface and its modification potential are of utmost interest for future large-scale production. This study focuses on two semiconducting Poly(3-hexylthiophene-2,5-diyl) diblock variants, whose sprayed and doped thin films show excellent potential as thermoelectric generators. Using AFM, ellipsometry, *in situ* GISAXS/GIWAXS, and NR measurements, the structural changes of the polymer-gold interfaces were tracked during thermal annealing.

CPP 36.7 Wed 16:45 GÖR 226

Compatible solution-processed interface materials for improving the efficiency of organic solar cells — •Zhuo Xu[1,2], Jose Prince Madalaimuthu[1,2], Josef Bernd Slowik[1,2], Rico Meitzner[1,2], Aman Anand[1,2], Shahidul Alam[1,2,4], Héctor Corte[5], Steffi Stumpf[1,3], Ulrich S. Schubert[1,2,3], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry, Friedrich Schiller University Jena, Jena, Germany. — [2]Center for Energy and Environmental Chemistry Jena, Friedrich Schiller University Jena, Jena, Germany. — [3]Jena Center for Soft Matter, Friedrich Schiller University Jena, Jena, Germany. — [4]King Abdullah University of Science and Technology, KAUST Solar Center, Physical Sciences and Engineering Division, Material Science and Engineering Program, Thuwal, Kingdom of Saudi Arabia. — [5]Nanosurf AG, Liestal, Switzerland.

The electron transport layer (ETL) is a key components for better performance and stability in OSCs. Herein, conjugated PDINO, sol-gel derivatized under stoichiometric TiOx, and the same combination as the ETL was used to fabricate solution-processed PBDTTT-C-T:PC71BM-based OSCs. A hybrid of organic-inorganic ETL revealed less bimolecular and trap-assisted recombination than a single ETL of either material. Furthermore, the efficiency of devices using blend ETLs showed better performance in comparison to single ETLs in both fullerene and non-fullerene systems. This blending strategy have demonstrated beneficial consequences in device stability and efficiency, which will play key role for future commercialization of OSCs.

CPP 36.8 Wed 17:00 GÖR 226

Influence of dye-doping on the nanostructure of the highly efficient PM6:Y6 solar cells — •Elisabeth Erbes[1,2], Constantin Harder[1,3], Benedikt Sochor[1], Susann Frenzke[1], Naireeta Biswas[1,2], Jan Rubek[1], Matthias Schwartzkopf[1], Volker Körstgens[3], Peter Müller-Buschbaum[3,5], Stephan V. Roth[1,4] und Simone Techert[1,2] — [1]DESY, Hamburg, DE — [2]Institute for X-ray Physics, Goettingen University, Goettingen, DE — [3]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [4]KTH Royal Institute of Technology, Stockholm, SWE. — [5]MLZ, TUM, Garching, DE

Organic solar cells based on the donor polymer PM6 and the acceptor Y6 give power conversion efficiencies (PCE) of 13-16% without any additives. The current study aims to investigate systematically the effect of doping PM6:Y6 with optical-light absorbing, electron transfer (ET) dyes. These pyrene-based dyes (PyxDMA) have inter- and intramolecular charge transfer properties and a very high quantum yield. Also the absorption in the UV regime extends the absorption range of the PM6:Y6 system. The structural and morphological integrity of the dopants within the active layer were studied with grazing incidence X-ray scattering experiments. The analysis showed the intercalation and distribution of the dyes within the PM6:Y6 matrix. The sprayed solar cell architecture Cu/PM6:Y6:PyxDMA/PEDOT:PSS/Au/ITO/Glass was used to measure the PCEs. Correlating these efficiencies with the molecular and nanostructural results allows explaining the changing PCE due to different doping levels of PyxDMA.

CPP 36.9 Wed 17:15 GÖR 226

Hydrogenated nanodiamonds as efficient electron extraction layers in organic solar cells — •Aurelien Sokeng Djoumessi[1,2], Anastasia Sichwardt[1,2], Daria Miliaieva[3], Jan Čermák[3], Maximilian Schaal[4], Felix Otto[4], Štěpán Stehlík[3], Vojtech Nádaždy[6], Torsten Fritz[4], Bohuslav Rezek[5], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry, Friedrich Schiller University Jena (IOMC), Jena, Germany — [2]Center for Energy and Environmental Chemistry (CEEC), Friedrich Schiller University Jena, Jena, Germany — [3]Institute of Physics, Czech Academy of Sciences, Prague 6, Czech Republic — [4]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [5]Faculty of Electrical Engineering, Czech Technical University, Prague, Czech Republic — [6]Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovak Republic

Surface tunability is one property of nanodiamonds (NDs), which enables to attachment of a range of functional groups on their surfaces. This may have a significant impact on NDs' electrical and optical characteristics and be helpful for charge extraction in solar cell devices. Herein, the surface chemistries of HPHT NDs modified by hydrogenation in a hydrogen atmosphere exhibit sp2-phases, which may help in improving the material's electrical conductivity and electron extraction when employed as an electron transport layer in PBDB-T:ITIC-based solar cells. The device performance was 7%, which differs only marginally from the outcomes of the state-of-the-art ETLs (ZnO, SnO2).

CPP 37: Nanostructures, Nanostructuring and Nanosized Soft Matter

Time: Wednesday 15:00–16:15 Location: MER 02

CPP 37.1 Wed 15:00 MER 02

Structure and dynamics of a 1,4-polybutadiene melt in an alumina nanopore: A molecular dynamics study — •Lama Tannoury[1], Mathieu Solar[2], and Wolfgang Paul[1] — [1]Martin-Luther-Universität Halle-Wittenberg — [2]Université de Strasbourg

The study of the structure and dynamics of polymer melts confined by solid surfaces enhances our knowledge about the glass transition temperature as well as that of composite materials. It has been shown that conformations and dynamics of polymer melts confined to thin films and flat surfaces as well as cylindrical pores are altered in comparison with the bulk. The change in properties depends on several factors including but not limited to the geometry of confinement. In this research, we study the effects of both nanoscopic confinement and curvature on the dynamics and properties of a chemically realistic 1,4-polybutadiene (PBD) melt using Molecular Dynamics (MD) simulations. We investigate the density layering across the nanopore as well as the orientational ordering in the melt on both the segmental and chain scales. As for the dynamics, we show that the confinement creates an adsorbed layer that not only slows down the relaxation but also creates a third step not present in the bulk. The system has also been investigated by different experimental techniques, allowing for a comparison of our simulations to the experimental data.

CPP 37.2 Wed 15:15 MER 02

Toluene-mediated morphology transition of amphiphilic diblock copolymer templated Si/Ge/C thin films — •Christian L. Weindl[1], Kexin Wu[1], Christian E. Fajman[2], Constantin Harder[3], Benedikt Sochor[3], Matthias Schwartzkopf[3], Stephan V. Roth[3,4], Thomas F. Fässler[2], and Peter Müller-Buschbaum[1,5] — [1]TUM School of Natural Sciences, Chair of Functional Materials, 85748 Garching — [2]TUM School of Natural Sciences, Chair of Inorganic Chemistry with Focus on Novel Materials, 85748 Garching — [3]DESY, 22607 Hamburg — [4]Royal Institute of Technology KTH, 100 44 Stockholm — [5]MLZ, TUM, 85748 Garching

The latest research has revealed promising results for silicon (Si) and germanium (Ge) as anode materials for lithium-ion batteries. These two group 14 semiconductors are considered auspicious additives in graphite anodes due to their high specific capacity (Si) and electron mobility (Ge). This study aims to synthesize a mesoporous Si/Ge/C structure over a wet chemical sol-gel approach with the structure-directing amphiphilic diblock copolymer PS-b-PEO and the Zintl cluster $K_{12}Si_xGe_{17-x}$. Furthermore, we added toluene as an additive to further induce the microphase separation. Real-space data as SEM will be discussed with the reciprocal-space analysis methods as grazing-incidence small/wide-angle x-ray scattering (GISAXS/GIWAXS). Finally, as an application, we will show the performance of these novel films as Li-ion battery anodes.

CPP 37.3 Wed 15:30 MER 02

Ultracompact Beam Deflector using Electrically Switchable Metallic Polymer Nanogratings — •Yohan Lee, Julian Karst, Monika Ubl, Mario Hentschel, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569, Stuttgart, Germany

We introduce nanogratings from metallic polymers which show an electrochemically-driven optical metal-to-insulator transition. A key feature of the design is separately addressable electrodes to vary the superlattice period of the grating via the applied voltages. Thus, the proposed ultracompact beam deflectors can generate various angles.

CPP 37.4 Wed 15:45 MER 02

Molecular dynamics of superglassy polymers for gas separation by neutron scattering, dielectric spectroscopy, and calorimetry — •Paulina Szymoniak[1], Mohamed Aejaz Kolmangadi[1], Reiner Zorn[2], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany — [2]Forschungszentrum Jülich, Jülich Centre for Neutron Science, Jülich, Germany

Janus polytricyclononenes (PTCN) with rigid backbones and flexible n-alkyl (n=propyl-decyl) are innovative materials that show potential in separating hydrocarbons. These superglassy polymers were designed to show an enhanced, controllable gas permeability via flexible alkyl side chains. PTCNs show nanophase separation between the alkyl side chains and the backbones with a distinct α-relaxation of the alkyl-rich nanophase found by broadband dielectric spectroscopy and temperature modulated DSC. Further, Janus PTCNs were studied by quasielastic neutron scattering (QENS) employing backscattering and time of flight instruments. For an overview of dynamic processes inelastic fixed window scans were performed showing segmental motions of alkyl-rich nanodomains and an additional low temperature relaxation, assigned to methyl group rotations. The molecular mobility was extracted from a combined analysis of backscattering and time of flight QENS data. The glass transition of the backbone-rich domains, which is beyond or near to the degradation of the materials, was evidenced by fast scanning calorimetry by decoupling it from decomposition, employing high heating rates.

CPP 37.5 Wed 16:00 MER 02

Size matters: Size Effects on Surface Chemistry and Raman Spectra of Sub-5 nm Oxidized High-Pressure High-Temperature and Detonation Nanodiamonds — •Bernhard Schummer[1] and Stepan Stehlik[2] — [1]Fraunhofer Development Center X-ray Technology, 90768 F*urth, Germany — [2]Institute of Physics of the Czech Academy of Sciences, 162 00 Prague 6, Czechia

Materials with very small dimensions of a few nanometers is of major importance for fundamental science as well as innovative applications. Those nanomaterials show different effects like quantum size effects, structural transformation or phonon-confinement effects. It has been predicted theoretically that nanodiamonds (NDs) have a structural transformation and phonon-confinement effect below 3 nm in size. Here, we investigate how size effects the surface chemistry, microscopic structure, and Raman scattering of high-pressure high-temperature (HPHT) and detonation nanodiamonds (DNDs) between 2 to 3 nm. The particle size and particle size distribution (PSD) of those different fractions was analyzed with dynamic light scattering, analytical ultracentrifugation, small-angle X-ray scattering, X-ray diffraction, and transmission electron microscopy as complementary techniques. Comprehensive comparison of detonation and pure monocrystalline HPHT NDs reveals effects of diamond core size and defects, chemical and temperature (in)stability, and limitations of current phonon confinement models.

CPP 38: Microswimmers and Fluid Physics of Life (joint session DY/CPP)

Time: Wednesday 15:00–18:15 Location: MOL 213

CPP 38.1 Wed 15:00 MOL 213

Physics of gut motility governs digestion and bacterial growth — •Agnese Codutti[1], Jonas Cremer[2], and Karen Alim[1] — [1]School of Natural Sciences, Technical University of Munich, Germany — [2]Biology Department, Stanford University, USA

Malfunctioning of the small intestine contractility and the ensuing bacterial population therein are linked to a plethora of diseases. We, here, study how the small intestine's variety of contractility patterns impacts nutrient uptake and bacterial population [1]. Our analytical derivations in agreement with simulations identify flow velocity as the key control parameter of the nutrients uptake efficiency and bacterial growth, independently of the specifics of contractility patterns. Self-regulating flow velocity in response to the number of nutrients and bacteria in the gut allows for achieving 100% efficiency in nutrient uptake. Instead of the specifics of intestine contractility, our work points to the flow velocity and its variation in time within the intestine to prevent malfunctioning.

[1] Codutti A., Cremer J., Alim K., "Changing Flows Balance Nutrient Absorption and Bacterial Growth along the Gut" PRL 129, 138101 (2022)

CPP 38.2 Wed 15:15 MOL 213

Turbulence induces clustering and arrested phase separation in polar active fluids — Vasco Worlitzer[1,2], Gil Ariel[2], Avraham Beer[3], Holger Stark[4], •Markus Bär[1,4], and Sebastian Heidenreich[1] — [1]Physikalisch-Technische Bundesanstalt, Berlin — [2]Bar-Ilan University, Ramat Gan, Israel — [3]Ben-Gurion University, Beer Sheva, Israel — [4]Technische Universität Berlin

We study a novel phase of active polar fluids, which is characterized by the continuous creation and destruction of dense clusters due to self-sustained turbulence. This state arises due to the interplay between self-advection of the aligned swimmers and their defect topology. The typical cluster size is determined by the characteristic vortex size. Our results are obtained by investigating a continuum model of compressible polar active fluids [1], which incorporates typical experimental observations in bacterial suspensions [2], in particular a non-monotone dependence of speed on density.

[1] V. Worlitzer et al., Soft Matter 17, 10447-10457 (2021)
[2] A. Beer et al., Communications Physics 3, 66 (2020)

CPP 38.3 Wed 15:30 MOL 213

Bacterial spreading in complex environments — •Agniva Datta, Sönke Beier, Veronika Pfeifer, Robert Grossmann, and Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany

Elucidating the principles of bacterial motility and navigation is key to understand many important phenomena such as the spreading of infectious diseases and the formation of biofilms. A prime challenge of swimming bacteria is to navigate in their habitat purposefully and efficiently, e.g., in the soil, which is a complex, structured environment. In this talk, we address the question of how bacterial navigation at the microscale relates to their large-scale spreading in heterogeneous environments. We combine experiments with the soil bacterium *Pseudomonas putida* with active particle modeling. In particular, the motility pattern of these bacteria in agar will be discussed with a focus on anomalous transport properties in disordered environments. In contrast to *E. coli*, our analysis reveals transient subdiffusion of bacteria in agar due to intermittent trapping, giving rise to a hop-and-trap dynamics with power-law distributed trap times.

CPP 38.4 Wed 15:45 MOL 213

Minimum Entropy Production by Microswimmers with Internal Dissipation — •Andrej Vilfan, Abdallah Daddi-Moussa-Ider, Babak Nasouri, and Ramin Golestanian — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Microswimmers are natural or artificial self-propelled microscale objects moving through a fluid at low Reynolds numbers. The entropy production of microswimmers, related to their dissipated power, consists of two contributions. The external dissipation takes place in the viscous fluid surrounding the microswimmer. Internal dissipation takes place in the propulsive layer on the swimmer's surface. We have previously shown that a lower bound on the external dissipation can be derived with the knowledge of drag coefficients of two bodies of the same shape, one with a no-slip and one with a perfect slip boundary condition [1]. Here, we show that our approach can be generalized to take into account the internal dissipation, which is often the dominant contribution. By combining the Helmholtz minimum dissipation theorem and the principle of linear superposition, we solve the combined minimum dissipation problem for different classes of swimmers including surface-driven viscous droplets, swimmers driven by tangential forces and swimmers driven by normal forces. We show that the minimum entropy production in suspensions of active microswimmers differs fundamentally from particles driven by external forces.

[1] B. Nasouri, A. Vilfan and R. Golestanian, Phys. Rev. Lett., 126, 034503 (2021).

CPP 38.5 Wed 16:00 MOL 213

Synchronization of model cilia by time-dependent elastohydrodynamics — •Albert von Kenne[1], Holger Stark[2], and Markus Bär[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), 10587 Berlin — [2]Technische Universität Berlin, 10623 Berlin

Collections of hair-like micro actuators known as cilia are employed in biology to pump extra cellular fluids at low Reynolds number conditions. Their collective dynamics exhibit synchronization and a large scale coordinated motion called metachronal waves. Typically, simple models that characterize the self-organization among hydrodynamically interacting cilia neglect the inertial forces in the fluid against the viscous forces. In this case, the mutual flows are determined instantaneously through the forces exerted by cilia. Consequentially synchronization requires a symmetry breaking external to hydrodynamics, that can come from elastic responses to flow perturbations (*T. Niedermayer et al., Chaos 2008*). Meanwhile, experiments show that inertial forces are significant in microscopic flow at the relevant scales (*D. Wei et al. Phys. Rev. Lett. 2019*). In this situation, the fluid response is explicitly time-dependent and hydrodynamic correlations can lead to synchronization (*M. Theers and R. Winkler, Phys. Rev. 2013*). We derived a simplified phase-oscillator model that describes the leading order coupling between cilia by elastic responses and hydrodynamic correlations. We show that its interrelations don't change the collective state qualitatively. However, the strength of coupling is always increased.

CPP 38.6 Wed 16:15 MOL 213

Microswimming near a wedge — •Alexander R. Sprenger and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany

Artificial and living microswimmer encounter a large variety of geometric confinements and surfaces in the biological world which alter their motion when nearby. Here, we study the low-Reynolds-number dynamics of a microswimmer enclosed by a wedge-shaped free-slip interface. For various opening angles of the wedge, we derive an exact solution for flow and pressure fields using the method of images. The active swimmer is represented in terms of a superposition of Stokes singularities. In this way, the hydrodynamic interactions between the swimmer and the confining interfaces are examined. In particular, we find attraction or repulsion by the wedge depending on the propulsion mechanism (pusher- or puller-type swimming strokes) and the opening angle of the wedge. For the dynamics of a microswimmer inside the wedge, we present a minimal model in terms of coupled Langevin equations for position and orientation. Our analytic results are evaluated for parameters inspired by common self-propelling microorganisms like *Escherichia coli.*

15 min. break

CPP 38.7 Wed 16:45 MOL 213

Role of cohesion in the flow of active particles through bottlenecks — •Timo Knippenberg[1], Anton Lüders[1], Celia Lozano[2], Peter Nielaba[1], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, Germany — [2]Bosonit, AI Department, La Rioja, Spain

Recently, many studies examined the intermittent flow of granular particles through bottleneck-shaped apertures. A common framework which describes the occurring flow statistics was empirically found for a wide range of such systems reaching from microscopic colloids and macroscopic grains up to sheep herds. However, similar studies with active matter are scarce and do merely consider steric agent interactions. Here, we experimentally and numerically study the flow of programmable, colloidal active Janus swimmers through bottlenecks. Our results confirm the applicability of the above-mentioned statistical framework of granular intermittent flow also on complex-interacting active microswimmers. Moreover, upon increasing the strength of interparticle cohesion, we find a transition from an arch-dominated clogging regime to a cohesion-dominated regime where droplets form at the outlet. The flow-rate only weakly depends on the cohesion strength in the arch-dominated regime, which suggests that cohesion needs not necessarily to hinder particle flow through geometric constrictions or pores.

CPP 38.8 Wed 17:00 MOL 213

Self-assembling meso-machines along liquid-air interfaces — •Nicolas Vandewalle, Megan Delens, and Ylona Collard — GRASP, University of Liege, B4000 Liege, Belgium

Magnetocapillary driven self-assembly allows us to create complex structures floating along a liquid-air interface. We show how these structures can be elaborated and how they can be triggered for locomotion. First, the pairwise capillary and magnetic interactions between floating objects are experimentally studied and rationalized through analogies with electrostatics. Then, the combination of capillary attraction and magnetic repulsion will lead to the spontaneous formation of a rich variety of floating structures. Placed in processing magnetic fields, those structures may behave like swimming ciliate organisms and start to move along the liquid-air interface. The conditions to obtain this magnetic powered locomotion are emphasized.

CPP 38.9 Wed 17:15 MOL 213

Induced capillary dipoles in floating particle assemblies — •Megan Delens, Ylona Collard, and Nicolas Vandewalle — GRASP, Institut de Physique B5a, Université de Liège, Liège, BE

Capillary-driven self-assembly is a common fabrication method that consists in placing floating particles onto a liquid-air interface. The attractive capillary interaction between particles is due to the local deformations of the interface which can be described via so-called capillary charges. When the particles are spherical and far from each other, the menisci are planar circles and can be described by monopolar capillary charges. The capillary interaction is then approximately found by assuming that the charges carried by individual spheres may be linearly superposed. However, when particles are close together, we experimentally observed that the attraction is enhanced and becomes far more complex. Indeed, the contact lines start to tilt and the superposition principle no longer holds. For these situations, we propose to additionally consider induced capillary dipoles to describe the menisci, therefore, providing an extra attraction between particles at short distances. This effect is enhanced when particles have different sizes such that binary self-assemblies may reveal unusual local ordering.

CPP 38.10 Wed 17:30 MOL 213

A Versatile Swarm of Individually Controlled Microparticles for Object Manipulation and Transport — •Veit-Lorenz Heuthe[1], Emanuele Panizon[2], and Clemens Bechinger[1] — [1]Universität Konstanz, Konstanz, Germany — [2]International Centre for Theoretical Physics, Trieste, Italy

Some tasks for robotic systems require many robots to cooperate, similar to ants that join their forces to carry large objects. On a macroscopic scale, many examples for such collective tasks exist, like robot swarms that can assemble objects. However, future potential applications like minimally invasive medicine call for miniaturization of such concepts. On the microscopic scale, one major challenge is the strong thermal noise, that demands for much more robust control. We use a reinforcement learning algorithm to individually steer microswimmers in a swarm that can manipulate and transport a large object. Due to decentralized control, our multi robot system is highly flexible, scalable and robust. With this demonstration we take micro-robot swarms one step further on their way to become tools for manipulating microscopic objects.

CPP 38.11 Wed 17:45 MOL 213

New insights into the mechanism of self-phoresis — •Alvaro Domínguez[1], Mihail Popescu[1], and Siegfried Dietrich[2] — [1]Univ. Sevilla, Spain — [2]MPI für Intelligente Systeme, Stuttgart

Chemophoresis describes the displacement of a particle in an ambient fluid due to a gradient in chemical composition. Classic phoresis can be understood through linear–response theory: in the presence of a sufficiently small gradient $(\nabla n)_{\mathrm{ext}}$ in concentration, the phoretic velocity of the particle is $\mathbf{V} = \mathcal{L}_{\text{lin}}(\nabla n)_{\text{ext}}$, in terms of the phoretic coefficient $\mathcal{L}_{\text{lin}}$ given by a Green–Kubo expression.

Self-phoretic particles induce a composition gradient $(\nabla n)_{\text{act}}$ through catalytic activity and provide a physical realization of artificial swimmers. Experimental observations are then customarily addressed as another instance of classic phoresis, $\mathbf{V} = \mathcal{L}_{\text{lin}}(\nabla n)_{\text{act}}$.

However, an additional role of the particle's chemical activity has been recently identified [1,2], namely, as responsible for a specific activity–induced response $\mathcal{L}_{\text{act}}$, so that one has to write

$$\mathbf{V} = (\mathcal{L}_{\text{lin}} + \mathcal{L}_{\text{act}})\,[(\nabla n)_{\text{ext}} + (\nabla n)_{\text{act}}]$$

in the more general scenario. This would mean a change in paradigm as it disproves the claim that "self-phoresis is phoresis in a self-induced gradient".

[1] A. Domínguez, M. Popescu, C. Rohwer, S. Dietrich, Physical Review Letters, **125**, 268002 (2020).

[2] A. Domínguez, M. Popescu, Current Opinion in Colloid & Interface Science, **61**, 101610 (2022).

CPP 38.12 Wed 18:00 MOL 213

Orientational dynamics and rheology of active suspensions in viscoelastic media — •Akash Choudhary[1], Sankalp Nambiar[2], and Holger Stark[1] — [1]Institute of Theoretical Physics, Technische Universität Berlin, 10623 Berlin, Germany — [2]KTH Royal Institute of Technology and Stockholm University, Stockholm 10691, Sweden

Active suspensions are systems of motile organisms or active filaments that are driven out of equilibrium through self-propulsion. This localized energy-work conversion imparts rich phenomenology and anomalous macroscale properties that are in stark contrast to passive suspensions and polymeric fluids. Motivated by the ubiquitous microbial systems in biological fluids, we analyse the impact of non-Newtonian fluids on the rheological response of active suspensions to steady shear flows.

We first study the suspension at an individual level and show that elongated pushers (representative of *E. coli*) and pullers (*C. reinhardtii*) exhibit diverse orbital dynamics in a weakly viscoelastic shear flow. We find that the active stresses not only modify the Jeffery orbits well-known from Newtonian fluids, but microswimmers can exhibit alignment and shear-plane rotation states. To analyze the impact of such behavior on the bulk rheological response, we study an ensemble of a dilute suspension of such swimmers in the presence of stochastic noise from bacterial tumbling and rotary diffusion. In comparison to Newtonian media, the polymeric elastic stresses substantially amplify the swimmer-induced viscosity, in particular, the superfluid transition observed in pusher solutions.

CPP 39: Focus Session: Physics of Fluctuating Paths (joint session DY/CPP)

State-of-the-art experiments probe physical observables, such as heat, work or entropy production, empirical densities and currents, on the level of individual, stochastic paths. Such experiments are typically analysed by averaging along a limited number of individual realisations, which leads to substantial uncertainties in estimates. The systematic sample-to-sample fluctuations of such path-observables encode important information about the underlying, microscopic dynamical processes and are therefore a frontier of experimental, theoretical, and computational physics. Recently there has been a surge in the development and applications of path-based concepts across many fields of physics. This focus session complements a symposium and contains contributed talks.

Organized by Aljaz Godec, Udo Seifert, and Peter Sollich

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

CPP 39.1 Wed 15:00 ZEU 160

Towards a stochastic thermodynamics of fields and tracers — •Sarah A.M. Loos[1], Davide Venturelli[2], Benjamin Walter[3], Edgar Roldan[4], and Andrea Gambassi[2] — [1]DAMTP, University of Cambridge, Cambridge, UK — [2]SISSA, Trieste, Italy — [3]Imperial College London, UK — [4]ICTP, Trieste, Italy

Many results of stochastic thermodynamics, including the close connection between entropy production and stochastic heat dissipation, rely on physical assumptions, e.g., break down if there is no clear separation into "fast equilibrium bath degrees of freedom" and "slow nonequilibrium degrees of freedom". In this talk, I will discuss some insights into thermodynamic notions of nonequilibrium systems that do not fall into the usual paradigm of stochastic thermodynamics. In particular, we develop a thermodynamic description for systems consisting of tracer particles coupled to correlated scalar fields with thermal fluctuations in terms of trajectory-wise energy flows of the particle and the field, as well as the joint entropy production rate measured by path-probability ratios. As an illustration, we consider the case in which the particle is dragged by a harmonic trap through a complex medium described by a fluctuating Gaussian field. Using a perturbative approach, we uncover three dynamical regimes with distinct scaling behavior of the power and discuss the heat dissipation occurring within the field.

CPP 39.2 Wed 15:15 ZEU 160

Fluctuation theorem for time reversal markers — •Gabriel Knotz, Till M. Muenker, Timo Betz, and Matthias Krüger — Fakultät für Physik, Georg-August-Universität, Göttingen, Germany

The analysis of particle trajectories is of high theoretical and experimental interest. Especially if hidden degrees are present, detecting broken detailed balance is a challenging task. We introduce and analyze a class of observables with certain symmetry properties under time reversal of trajectories that detect the breakage of detailed balance. Further, these observables fulfill a new form of fluctuation theorem and, under certain conditions, this fluctuation theorem provides bounds and relations for the total change in entropy. These findings are not limited to Markov or overdamped dynamics.

CPP 39.3 Wed 15:30 ZEU 160

Necessity for Coarse Graining Empirical Densities and Currents in Continuous Space — •Cai Dieball and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Goettingen, Germany

We present general results on fluctuations and spatial correlations of the coarse-grained empirical density and current of diffusion in equilibrium or non-equilibrium steady states on all time scales. The time averaging and coarse graining hardwired in the definition of the functionals under consideration give rise to experimentally relevant but highly non-trivial statistics. We unravel a deep connection between current fluctuations and generalized time-reversal symmetry. We highlight the essential role of coarse graining in space from mathematical, thermodynamical, and experimental points of view. Spatial coarse graining is required to uncover salient features of currents that break detailed balance, and a thermodynamically "optimal" coarse graining ensures the most precise inference of dissipation. Defined without coarse graining, the fluctuations of empirical density and current are proven to diverge on all time scales in dimensions higher than one, which has far-reaching consequences for large-deviation limits in continuous space and for continuum limits of Markov-jump processes. Our findings provide new intuition about time-averaged observables and allow for a more efficient analysis of single-molecule experiments.

References: Phys. Rev. Lett. 129, 140601 (2022) and Phys. Rev. Research 4, 033243 (2022)

CPP 39.4 Wed 15:45 ZEU 160

How Stickiness Can Speed Up Diffusion in Confined Systems — Arthur Alexandre[1], Matthieu Mangeat[2], •Thomas Guérin[1], and David Dean[1] — [1]Laboratoire Ondes et matière d'Aquitaine, CNRS/University of Bordeaux, F-33400 Talence, France — [2]Center for Biophysics and Department for Theoretical Physics, Saarland University, D-66123 Saarbrücken, Germany

The paradigmatic model for heterogeneous media used in diffusion studies is built from reflecting obstacles and surfaces. It is well known that the crowding effect produced by these reflecting surfaces slows the dispersion of Brownian tracers. In this talk, using a general adsorption desorption model with surface diffusion, we present an analytical theory showing that making surfaces or obstacles attractive can accelerate dispersion. In particular, we show that this enhancement of diffusion can exist even when the surface diffusion constant is smaller than that in the bulk. Even more remarkably, this enhancement effect occurs when the effective diffusion constant, when restricted to surfaces only, is lower than the effective diffusivity with purely reflecting boundaries. We give analytical formulas for this intriguing effect in periodic arrays of spheres as well as undulating microchannels. Our results are confirmed by numerical calculations and Monte Carlo simulations. [Ref: How Stickiness Can Speed Up Diffusion in Confined Systems, Phys Rev Lett 128 210601 (2022)]

CPP 39.5 Wed 16:00 ZEU 160

From trajectories to models: data-driven approaches to decipher the stochastic dynamics of living systems — •Pierre Ronceray — Turing Centre for Living Systems, CINaM, CNRS, Aix-Marseille University, France

Stochastic differential equations are often used to model the dynamics of living systems, from Brownian motion at the molecular scale to the dynamics of cells and animals. How does one learn such models from experimental data? This task faces multiple challenges, from information-theoretical limitations to practical considerations. I will present a recent and ongoing effort to develop new methods to reconstruct such stochastic dynamical models from experimental data, with a focus on robustness and data efficiency. This provides a generic means to quantify complex behavior and unfold the underlying mechanisms of an apparently erratic trajectory.

CPP 39.6 Wed 16:15 ZEU 160

Entropons as vibrational excitations in active solids — •Lorenzo Caprini[1], Umberto Marini Bettolo Marconi[2], Andrea Puglisi[3], and Hartmut Löwen[1] — [1]Heinrich-Heine-Universität Düsseldorf — [2]Scuola di Scienze e Tecnologie, University of Camerino — [3]Istituto dei Sistemi Complessi, CNR

We study the vibrational properties of non-equilibrium active crystals, i.e. solids formed by active particles, that are intrinsically out of equilibrium and governed by entropy production. As known in solid-state physics, equilibrium crystals are characterized by basic collective excitations with thermal origins that are named phonons. In this talk, I will show that active crystals are described by additional vibrational excitations that we called 'entropons' because each of them represents a mode of spectral entropy production. Entropons coexist with phonons and dominate over them for large activity, i.e. when the solid is far from equilibrium, while they vanish in equilibrium conditions. Their existence can be verified in experiments on dense self-propelled colloidal Janus particles and granular active matter, as well as in living systems such as dense cell monolayers.

15 min. break

CPP 39.7 Wed 16:45 ZEU 160

Inferring Fractional Processes Using Path Integrals — •Johannes A. Kassel[1], Benjamin Walter[2], and Holger Kantz[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Imperial College London, London, UK

We present a method for inferring overdamped nonlinear Langevin equations driven by multiplicative fractional Gaussian noise from single-trajectory time series. Constructing a maximum-likelihood estimator, we simultaneously infer the nonlinear deterministic force term and the space-dependent diffusion term. We illustrate our method using artificial time series. We observe that Markovian modeling of long-range correlated data leads to a substantial underestimation of the deterministic force term while for anti-correlated data it leads to an overestimation of the force term.

CPP 39.8 Wed 17:00 ZEU 160

Kinetics of Imperfect Reactions for non-Markovian Random Walks — •Toni Vieira Mendes and Thomas Guérin — Laboratoire Ondes et Matière d'Aquitaine, Université de Bordeaux

Most transport influenced reactions between two random walkers are usually imperfect, i.e., they do not occur at first contact between the reactants. For such imperfect reactions, recent work has been made to determine the statistics of first reaction time for Markovian random walkers in confinement. However, a lot of physical random walks are actually non-Markovian, i.e., their movement in the future depend on the trajectory they have followed up to then, thus displaying memory effects. These memory effects can be seen, for example, for beads moving inside complex fluids where the force fields do not equilibrate instantly. In this contribution, we describe an analytical theory giving access to the mean reaction time for imperfect reactions for random walkers with memory in confinement. Our theory clearly shows that, contrary to the Markovian case, the reaction time is not the sum of the mean first passage time and the time to react once within reactive distance. We show that the results of our theory match the results of simulations for both one and two dimensions. Then, the equations are analytically solved in the limit of weakly non-Markovian processes. Remarkably, in the limit of weakly reactive targets for fractional Brownian Motion, we find that the mean reaction time displays a non-trivial scaling as a function of the reactivity.

CPP 39.9 Wed 17:15 ZEU 160

Instantons and the Path to Intermittency in Turbulent Flows — •André Fuchs[1], Corentin Herbert[2], Joran Rolland[3], Matthias Wächter[1], Freddy Bouchet[2], and Joachim Peinke[1] — [1]Institute of Physics and ForWind, University of Oldenburg, Küpkersweg 70, 26129 Oldenburg, Germany — [2]Université de Lyon, Ens de Lyon, Université Claude Bernard, CNRS, Laboratoire de Physique, F-69364 Lyon, France — [3]Université de Lille, CNRS, ONERA, Arts et Métiers Institute of Technology, Centrale Lille, UMR 9014 - LMFL - Laboratoire de Mécanique des fluides de Lille - Kampé de Fériet, F-59000 Lille, France

Processes leading to anomalous fluctuations in turbulent flows, referred to as intermittency, are still challenging. We consider cascade trajectories through scales as realizations of a stochastic Langevin process for which multiplicative noise is an intrinsic feature of the turbulent state. The trajectories are conditioned on their entropy exchange. Such selected trajectories concentrate around an optimal path, called instanton, which is the minimum of an effective action. The action is derived from the Langevin equation, estimated from measured data. In particular instantons with negative entropy pinpoint the trajectories responsible for the emergence of non-Gaussian statistics at small-scales.

CPP 39.10 Wed 17:30 ZEU 160

A nonadiabatic generalized-dividing-surface instanton rate theory — •Rhiannon A. Zarotiadis, Joseph E. Lawrence, and Jeremy O. Richardson — Lab. für Physikalische Chemie, ETH Zürich, Zürich, Switzerland.

The accurate prediction of quantum rate processes is fundamental to our understanding of chemical reactions, but exact calculations are extremely costly. To make them tractable many chemical processes are described within the Born-Oppenheimer (BO) approximation, which assumes strong coupling between the diabatic states, and BO instanton theory is known to capture nuclear quantum effects for these systems well [1]. Alternatively, some systems are better captured by Fermi's golden rule, which is appropriate in the opposite limit of weak coupling.

Nevertheless, many reactions are in neither of these two limits, and so a universal rate theory is desirable. We introduce a new nonadiabatic generalized-dividing-surface instanton approach rigorously derived from the flux-flux correlation function. Our new theory correctly recovers the weak- and strong-coupling limits and goes beyond existing, ad hoc attempts to describe general, nonadiabatic rate processes.

Instanton rate theories [1] have already resolved many longstanding discrepancies between experiment and theory [2] and this new rate theory will be key to address processes beyond their scope such as proton-coupled electron transfer reactions.

[1] Richardson, J. O., Int. Rev. Phys. Chem., 2018, 37:2, 171-216.

[2] Zarotiadis, R. A., Fang, W., Richardson, J. O., Phys. Chem. Chem. Phys., 2020, 22, 10687.

CPP 39.11 Wed 17:45 ZEU 160

Sojourn probabilities for diffusive dynamics with state-dependent friction: Theory and experiment — Alice Thorneywork[1,2], Jannes Gladrow[2,3], Ulrich F. Keyser[2], Ronojoy Adhikari[4], and •Julian Kappler[4,5] — [1]Department of Chemistry, University of Oxford, Oxford, United Kingdom — [2]Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom — [3]Microsoft Research, Cambridge, United Kingdom —

[4]Department of Applied Mathematics and Theoretical Physics, Cambridge University, Cambridge, United Kingdom — [5]Fakultät für Physik, Ludwig-Maximilians-Universität, München, Germany

The trajectories of diffusion processes are continuous but nondifferentiable, and each occurs with vanishing probability. This introduces a gap between theory, where path probabilities are used in many contexts, and experiment, where only events with nonzero probability are measurable. We bridge this gap by considering the sojourn probability, i.e. the probability for diffusive trajectories to remain within a tube of small but finite radius around a smooth path. For systems with state-dependent diffusivity, we show that the sojourn probability is characterized by a functional that is different from all previously reported multiplicative-noise stochastic actions. We corroborate our theoretical results by comparison to experimentally measured sojourn probabilities for a colloidal particle in a corrugated microchannel. Our work directly connects the discussion of path probabilities for diffusive dynamics with state-dependent friction to physical observables.

CPP 39.12 Wed 18:00 ZEU 160

Optimality of non-conservative driving in discrete systems — •Jonas Fritz and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

A fundamental problem in stochastic thermodynamics is that of optimal driving. The goal is to drive a system from some specified initial state to a specified final state, while minimizing entropy production (or work performed) along the trajectory. As shown recently [1], the optimal protocol in a cyclical Markov network has a non-conservative force, i.e. non-zero cycle affinity, which is in contrast to continuous systems. However, the reduction in entropy production from such a non-conservative force has been numerically found to be at most on the order of 10^{-2} for the case of the three state cycle. We investigate why this is the case, by systematically varying step size and initial conditions numerically for the simple case of the three state cycle. Further, we try to maximize the improvement in entropy production through the non-conservative force. By increasing the number of states in the cycle, we find a possible improvement which is an order of magnitude larger than the previously known one. We attempt to find a lower bound for the possible improvement through non-conservative driving, by analyzing the scaling behavior of the underlying quantities.

[1] Benedikt Remlein and Udo Seifert, Phys. Rev. E 103, L050105

CPP 40: 2D Materials V: Growth, Structure and Substrate Interaction (joint session O/CPP)

Time: Wednesday 15:00–17:30 Location: GER 37

CPP 40.1 Wed 15:00 GER 37

Te on Pt(111): Structure and Growth of Surface Tellurides and $\mathbf{Pt}_x\mathbf{Te}_y$ Films — Tilman Kisslinger, Alexandra Schewski, Andreas Raabgrund, Hannah Loh, Lutz Hammer, and •M. Alexander Schneider — Lehrstuhl für Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

By LEED-IV, STM and DFT we investigated the tellurization of Pt(111) in UHV. For Te coverages $\Theta < 0.5\,\mathrm{ML}$ surface tellurides are formed. In this coverage regime and after thermal annealing, we find only two well ordered surface telluride structures with (3×3) and (10×10) periodicity, the former was mistaken for a defective $PtTe_2$ film [1]. Our LEED-IV structure analyses determine the atomic structure and show that the Pt(111) surface undergoes massive reconstructions upon reaction with Te.

For $\Theta > 0.5\,\mathrm{ML}$, compact islands develop which eventually coalesce to a complete platinum telluride layer. Again by LEED-IV analyses we find that the first layer is a Pt_2Te_2 layer on which as second layer a $PtTe_2$ film can be grown. Both form an overlayer where 7×7 film unit cells lie on 10×10 Pt(111) unit cells. Furthermore, we find that the interface to the Pt(111) bulk still contains the $\approx 0.5\,\mathrm{ML}$ Te originally bound in the (10×10) superstructure. Electronic properties of the films determined by STS and implications for the MBE growth of transition metal dichalcogenides by surface tellurization will be discussed.

[1] L. Liu, D. Zemlyanov, and Y.P. Chen, 2D Mater. **8**, 045033 (2021)

CPP 40.2 Wed 15:15 GER 37

Electronic, chemical and structural properties of ultrathin $\mathbf{Ta_2NiSe_5}$ flakes — •Kathrin Küster[1], Yuanshan Zhang[1], Dennis Huang[1], Ulrich Starke[1], and Hidenori Takagi[1,2,3] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, 70569 Stuttgart, Germany — [3]Department of Physics, University of Tokyo, 113-0033 Tokyo, Japan

The excitonic insulator is a theoretically proposed state of matter wherein a macroscopic condensate of electron-hole pairs, i.e., excitons, spontaneously forms below a transition temperature. The 2D-layered chalcogenide Ta_2NiSe_5 has arisen as a leading candidate of an excitonic insulator in a bulk crystal. Here we prepared ultrathin films (down to 2 nm) of Ta_2NiSe_5 and analyzed their structural, electronic and chemical properties with a NanoESCA (Scienta Omicron) on a local scale. Angle-resolved photoelectron spectroscopy (ARPES), X-ray photoelectron spectroscopy (XPS), together with photoelectron emission microscopy (PEEM) and imaging XPS give detailed insight into the thickness dependent properties of the flakes. By exposure to UV-light we observe a contrast change in the PEEM images which is caused by a strong modification of the work function of the flakes, which we tentatively relate to a phase transition of the Ta_2NiSe_5 flakes.

CPP 40.3 Wed 15:30 GER 37

Transition from fractal-dendritic to compact islands for the 2D-ferroelectric SnSe on graphene/Ir(111) — Paulus Aleksa, Sammer Iqbal, Muhammad Ali Martuza, Jiaqi Cai, Thais Chagas, Robin Ohmann, and •Carsten Busse — Universität Siegen, Germany

Monolayer islands of the 2D-ferroelectric SnSe have been grown by MBE under UHV conditions using inert and weakly interacting graphene on Ir(111) as the substrate. After deposition at room temperature, fractal-dendritic islands are observed in STM. The preferential growth directions are aligned with high-symmetry directions of the substrate. Upon annealing the islands become more compact. At 560 K they exhbit their equilibrium shape, higher temperatures lead to desoprtion. The equilibrium shape cannot be simply explained by minimization of the number of unsaturated bonds around the perimeter of an island with given area. The model has to be extended to incorporate the polar character of SnSe, leading to island edges that are charged in dependence of their orientation.

CPP 40.4 Wed 15:45 GER 37

Reaction of submonolayer amounts of Ti and Te on Au(111) — •Andreas Raabgrund, Tilman Kisslinger, Lutz Hammer, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Titanium ditelluride ($TiTe_2$) belongs to the family of layered 2D transition metal dichalcogenides. It achieved a lot of attention due to the emergence of a charge density wave in the single layer limit. Thicker films, however, do not show this transition [1]. Aiming the MBE growth of $TiTe_2$ we investigated the initial growth of titanium telluride structures on Au(111) both structurally and electronically by STM, STS, LEED-IV structural analysis, and DFT. For a Te coverage of 0.4 ML and a Ti coverage of 0.2 ML on Au(111) a chain-like $(5 \times \sqrt{3})_{\mathrm{rect}}$ superstructure is formed. Our LEED-IV best-fit structure with a Pendry R factor of 0.11 (redundancy $\rho = 9.6$) reveals incorporated Ti atoms each of which forms bonds to two Te atoms residing in approximately hollow positions. Our findings regarding the $(5 \times \sqrt{3})_{\mathrm{rect}}$ superstructure disprove the proposed $TiTe_2$ monolayer on Au(111) [2]. STS shows an approximately 0.5 eV (FWHM) wide peak at +1 V which we can correlate to the density of Ti d-states as obtained from DFT.

[1] P. Chen et al., Nat. Commun. **8**, 516 (2017)

[2] Z. Song et al., Chin. Phys. B **102**, 056801 (2019)

CPP 40.5 Wed 16:00 GER 37

Monolayers of $\mathbf{CoCl_2}$ and $\mathbf{CoBr_2}$ on Au(111) - Chemical, magnetic and structural investigation — •Samuel Kerschbaumer[1], Sebastien Hadjadj[2], Andrea Aguirre Baños[3], Danilo Longo[3], Wolfgang Kuch[2], José Ignacio Pascual[3], Celia Rogero[1], and Maxim Ilyn[1] — [1]Centro de Fisica de Materiales (CSIC/UPV-EHU), 20018 Donostia-San Sebastian, Spain — [2]Institut für Experimentalphysik, Freie Universität Berlin, 14195 Berlin, Germany — [3]CIC nanoGUNE-BRTA, 20018 Donostia-San Sebastian, Spain

Magnetic 2D materials have gained increasing interest, due to their potential applications. But while many theoretical calculations predict magnetic order in various 2D materials [1], only few have been experimentally measured [2]. A very promising classes of materials are transition metal halides (TMHs), as many of them crystallise in Van der Waals layered structures, making them easily cleavable, while their partially filled d orbitals generate the perfect foundation for magnetic order, further increasing their attractiveness for future nanotechnologies. In this talk chemical, magnetic and structural properties of single-layer $CoCl_2$ and $CoBr_2$ on Au(111) by scanning tunelling microscopy (STM), X-ray photoelectron spectroscopy (XPS), low energy electron diffraction (LEED) and X-ray absorption spectroscopy (XAS/XMCD) will be presented.

[1] Michael A. McGuire, Crystals, 7(5), 121, (2017)

[2] Djuro Bikaljevic et al., ACS Nano, 15, 14985 (2021)

CPP 40.6 Wed 16:15 GER 37

Structure determination of mono- and few-layers of the 2D-ferroelectric SnSe on graphene on Ir(111) — •Dina Wilks[1], Paulus Aleksa[1], Simon Chung[2], Peter Modregger[1], Dmitri V. Novikov[3], Vedran Vonk[2], Andreas Stierle[2,4], and Carsten Busse[1] — [1]Physics Department, University of Siegen, Germany — [2]Nanolabor Centre for X-ray and Nano Science CXNS, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Germany — [4]Physics Department, University of Hamburg, Germany

For conventional ferroelectrics the critical temperature T_c quickly falls below technically feasible values for very thin films. This is not the case for two-dimensional materials. Theory predicts strong ferroelectricity for group-IV monochalcogenides, where individual layers are puckered sheets with a phosphorene-like structure. For SnSe, stable ferroelectricity of monolayers at room temperature has been shown by controlled microscopic manipulation. Here, we provide the missing structure determination of these monolayers.

We use surface X-ray diffraction to determine the structure of SnSe mono- and few-layers, the influence of the substrate, and the difference in stacking between a few-layered system and the bulk. SnSe films are prepared by MBE using graphene on Ir(111) as an inert and weakly interacting substrate. We observe one phase with three different orientations of monolayer SnSe islands with respect to graphene, while for the few-layered system two phases are found, each with three different orientations. A change in structure with rising temperature for both systems is seen, which hints towards T_c.

CPP 40.7 Wed 16:30 GER 37

Electronic properties of epitaxially grown monolayer and bilayer VS_2 on Au(111) — •Mikhail Fonin[1], Sabina Simon[1], Felix Förschner[1], Jannik Dornseiff[1], Julia Tesch[1], Elena Voloshina[2], and Yuriy S. Dedkov[2] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Department of Physics, Shanghai University, 99 Shangda Road, 200444 Shanghai, China

Electronic properties of metallic two-dimensional materials can be strongly influenced by the supporting substrates, upon charge transfer or hybridization effects. In this context, suppression of many-body states in metallic transition metal dichalcogenides epitaxially grown on metallic substrates was recently reported [1]. By combination of scanning tunneling microscopy and first principle calculations we study monolayers and bilayers of VS_2 epitaxially grown on Au(111). We investigate the electronic properties of the monolayer and observe a metallic state with the presence of the incommensurate charge density wave state. Going form monolayer to bilayer VS_2, we observe an evolution from the metallic state to an insulating state.

[1] C. E. Enders *et al.,* Phys. Rev. B 94, 081404(R) 2016.

CPP 40.8 Wed 16:45 GER 37

Vanadium sulphides on graphene on Ir(111): polymorphs, charge density waves, layer dependency — •Camiel van Efferen[1], Joshua Hall[1], Virgínia Boix[2], Tobias Wekking[1], Nikolay Vinogradov[3], Alexei Preobrajenski[3], Jan Knudsen[2], Jeison Fischer[1], Wouter Jolie[1], and Thomas Michely[1] — [1]Universität zu Köln — [2]Lund University — [3]MAX IV Laboratory

Among 2D materials, vanadium based compounds like VS_2 have attracted substantial research interest due to their predicted electronically correlated and magnetic ground states. However, the charge density wave (CDW) in monolayer (ML) VS_2 and VSe_2 competes with predicted magnetic ground states. This has led to new research directions attempting to unlock the magnetic moment of the V atoms, e.g. via defect creation, alloying or the intercalation of atoms between VS_2 layers.

Here, we present a comprehensive X-ray photoemission spectroscopy and scanning tunneling microscopy study of few-layer, quasi-freestanding V_4S_7 and V_5S_8 on Gr/Ir(111), which are created via annealing of stoichiometric VS_2. Annealing ML VS_2 without background S pressure removes S atoms from the top layer of VS_2, creating the striped compound V_4S_7. In contrast, annealing ML VS_2 in a S atmosphere forms V_5S_8, where V atoms have self-intercalated between the VS_2 layers in a 2×2 pattern. Surprisingly, we find that V_5S_8 has a layer-dependent CDW at low temperature, with bilayer V_5S_8 exhibiting a $\sqrt{3} \times \sqrt{3}$ CDW, while the trilayer hosts a striped CDW phase akin to that of ML VS_2.

CPP 40.9 Wed 17:00 GER 37

Nucleation stage for the oriented growth of tantalum sulfide monolayers on Au(111) — •Thais Chagas[1], Kai Mehlich[1], Abdus Samad[2], Catherine Grover[1], Daniela Dombrowski[1,3], Jiaqi Cai[1], Udo Schwingenschlögl[2], and Carsten Busse[1] — [1]Department Physik, Universität Siegen, Siegen, Germany — [2]Physical Science and Engineering Division, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia — [3]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Münster, Germany

We study the nucleation stage in the epitaxial growth of monolayer TaS_2 as a model system for monolayer transition metal sulfides. The growth was done under ultra-high vacuum conditions with Au(111) as a substrate on which the metal atoms are evaporated, and the sulfur is provided from a background of H_2S. Using scanning tunneling microscopy (STM), we find small trimers with a well-defined triangular shape that act as nuclei for the further growth of extended tantalum sulfide monolayers. We identify these trimers as TaS_3 using density functional theory (DFT). We propose that the unique orientation of the trimers is the cause of the well-defined orientation of a complete TaS_2 layer found under favorable growth conditions.

CPP 40.10 Wed 17:15 GER 37

Growth and structure of two-dimensional single-layer HfS_2 on Au(111) — •Monika Schied, Paolo Lacovig, and Silvano Lizzit — Elettra-Sincrotrone Trieste

HfS_2 is a promising 2D material for low-power semiconductor devices due to its predicted high electron mobility and low contact resistance for n-type carrier transport. For actual applications, layers with excellent structural and electronic properties are needed. However, films with the necessary quality are only available from exfoliation, which is neither scalable nor very reproducible and only few experimental studies on a single-layer (SL) of HfS_2 have been performed so far. In analogy to the growth of high-quality SL transition metal dichalcogenides (TMDCs) such as MoS_2 and WS_2 [1,2] we have epitaxially grown an ordered layer of HfS_2 on Au(111) by chemical vapour deposition (CVD). Monitoring the S 2p and Hf 4f core levels in real time by fast X-ray photoelectron spectroscopy (XPS) allows the fine-tuning of the relevant parameters – such as the dosing rate and temperature – during the growth. The characterization by X-ray photoelectron diffraction (XPD) and low-energy electron diffraction (LEED) gives insight into the crystal structure of the film grown in this way.

[1] Bana, H., et.al., 2D Mater. 5 035012 (2018)

[2] Bignardi, L. et.al., Phys. Rev. Mat. 3, 014003, (2019)

CPP 41: Biopolymers, Biomaterials and Bioinspired Functional Materials II (joint session CPP/BP)

Time: Wednesday 16:30–18:00 Location: MER 02

CPP 41.1 Wed 16:30 MER 02

Low-Temperature and Water-Based Biotemplating of Nanostructured Foam-Like Titania Films using ß-Lactoglobulin — •Julian E. Heger[1], Wei Chen[1], Shanshan Yin[1], Nian Li[1], Volker Körstgens[1], Calvin J. Brett[2,3], Wiebke Ohm[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]DESY, Hamburg, Germany — [3]Royal Institute of Technology KTH, Stockholm, Sweden — [4]MLZ, TUM, Garching, Germany

Energy-related applications such as solar cells, batteries, and the photocatalytic production of hydrogen are broadly built up on titania nanostructures. A tailored titania morphology is necessary to match the required charge diffusion lengths and the crystallinity beneficial for efficient performance. In the context of large-scale fabrication, the aspect of sustainability becomes essential. Biopolymer templating based on ß-Lactogobulin (ß-lg) and spray deposition promotes low-temperature and water-based synthesis of nanostructured, crystalline, foam-like titania films. During spray deposition, the ß-lg biopolymer matrix sterically directs the titania morphology. Afterwards, the biotemplate is removed by UV-light exposure. To understand the kinetics of film formation during the spray deposition on the nano and crystalline length scale, we simultaneously perform in situ grazing-incidence small-angle and wide-angle X-ray scattering (GISAXS/GIWAXS). Together with scanning electron microscopy (SEM), the results explain the role of ß-lg as a biotemplate.

CPP 41.2 Wed 16:45 MER 02

Structural changes in cellulose nanofibril-colloid hybrid films during humidity cycling — •Stephan V. Roth[1,2], Calvin J. Brett[1,2], Alexandros Alexakis[2], Lucas P. Kreuzer[3], Martin Mansson[2], Sarah Rogers[4], Eva Malmström[2], Peter Müller-Buschbaum[3,5], and L. Daniel Söderberg[2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]KTH Royal Institute of Technology, Stockholm, Sweden — [3]TUM School of Natural Sciences, Chair for Functional Materials, Garching — [4]ISIS-STFC, Rutherford Appleton Laboratory, Chilton, Oxon OX11 0QX, UK — [5]MLZ, TUM, Garching, Germany

Biocompatible cellulose nanofibrils (CNFs) are an ideal material for sustainable biomaterial templates. Combined with latex colloids, the resulting hybrid colloid-CNF functional materials are excellent candidates for bio-inspired structural colors. Due to the hydrophilic nature of CNFs, we investigate the stability against humidity cycling in terms of reversible/irreversible structural rearrangements. We applied depth sensitive grazing incidence small-angle neutron scattering to evaluate the humidity-induced rearrangements in hybrid latex colloid:CNF templates in situ during cyclic humidification. After the first humidity cycle, a change in morphology on the scale of several 10 nm was observed, which is attributed to latex particles which diffused in the network and enlarged the pores of the network. The measured kinetics resolve the time- and depth-dependence of the differently sized colloids' penetration into the porous CNF network.

CPP 41.3 Wed 17:00 MER 02

Fluorescence correlation spectroscopy for studying the aggregation of nanoplastics in model biofilm substances — •Tobias Guckeisen, Rozalia Orghici, and Silke Rathgeber — Universität Koblenz, Deutschland

Nanoplastics in the environment are a growing problem. Pollutants can adhere to their surfaces and therefore be easily transported into the natural systems. Biofilms are found everywhere in the environment; they are formed by microbial communities that produce a matrix of extracellular polymeric substances. The interaction between nanoplastics and biofilms can lead to aggregation and sedimentation of nanoparticles and determines the transport and fate of nanoplastics. A better understanding of the transport and fate of nanoplastics is important to improve our ability to predict risks associated with these ubiquitous contaminants. In this project, we use fluorescence correlation spectroscopy (FCS) to study the aggregation and interactions of nanoplastics with model biofilm substances. Protein-polysaccharide mixing ratio and pH-dependent aggregation studies show that it is crucial to consider correlative effects between multiple biofilm components to better understand the impact biofilms have on nanoplastic aggregation. Biofilm model systems with only one component, as commonly considered, may lead to an incorrect assessment of the tendency to aggregation.

CPP 41.4 Wed 17:15 MER 02

Ensemble inequivalence and negative extensibility in a wormlike chain with fluctuating bending stiffness — •Panayotis Benetatos — Department of Physics, Kyungpook National University, Republic of Korea

Many semiflexible polymers exhibit fluctuations in the local bending stiffness along their contour. This may be due to intrinsic conformational changes (e.g., denaturation bubble formation in double stranded DNA or helix-coil transition in polypeptides) or to the reversible adsorption and desorption of molecules from the polymer's environment. In this presentation, we analyse the tensile elasticity of a strongly stretched wormlike chain which consists of N concatenated segments, where each segment can be in one of two states, A and B, which differ in bending stiffness. We call this model the reversible wormlike chain (rWLC) model. In the Gibbs (fixed-force, isotensional) ensemble, we obtain analytic expressions for the force-expression relation and the mean fraction of B segments. We show that, under certain conditions, there is a tension-induced crossover from a mostly A to a mostly B rWLC. In the Helmholtz (fixed-extension, isometric) ensemble, we obtain analytic expressions up to a summation. We show that, for finite N, there is marked ensemble inequivalence. Remarkably, in the Helmhlotz ensemble, the rWLC can exhibit negative extensibility and multiple peaks.

CPP 41.5 Wed 17:30 MER 02

Aging and compressed exponential stress relaxation in mechanoresponsive hydrogels — •Geonho Song[1,2], Wouter Ellenbroek[3], and Kerstin Blank[1,2] — [1]Johannes Kepler University Linz, Linz, Austria — [2]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [3]Eindhoven University of Technology, Eindhoven, The Netherlands

Biological materials, such as the extracellular matrix (ECM), are viscoelastic and exhibit stress relaxation. Stress relaxation in the ECM is linked to cellular behavior and needs to be considered as a design parameter when developing bioinspired materials for cell culture and tissue engineering. Here, we introduce a collagen-inspired hydrogel with tunable crosslink kinetics. We utilize collagen-mimetic peptides with controlled association and dissociation rates to crosslink star-shaped polyethylene glycol. We show that ultraslow crosslink dissociation rates cause a distinctive relaxation behavior that is reminiscent of soft glassy materials, showing out-of-equilibrium properties. In particular, subjecting the networks to a sequence of pre-stress and aging causes uncommon compressed exponential relaxation. This unique phenomenon has previously only been reported for a small number of soft glassy systems where compressed exponential relaxation was related to ultraslow dynamics that prohibited the release of internal stresses. In such systems, slow crosslink dissociation delays network relaxation until an external trigger is applied. In future work, we aim to investigate the interplay between locally generated stresses, such as cellular traction forces, and network relaxation properties.

CPP 41.6 Wed 17:45 MER 02

Nonaffinity controls critical slowing down and rheology near the onset of rigidity — •Abhinav Sharma[1], Jordan Shivers[2], and Fred MacKintosh[2] — [1]Leibniz institute for polymer research, Dresden — [2]Rice University, Houston, Texas

Fluid-immersed networks and dense suspensions often reside near a boundary between soft (or fluid-like) and rigid (or solid-like) mechanical regimes. This boundary can be crossed either by varying the concentration or by deformation. Near the onset or loss of rigidity, dissipation-limiting nonaffine rearrangements dominate the macroscopic viscoelastic response, giving rise to diverging relaxation times and power-law rheology. Here, we derive a simple relationship between nonaffinity and excess viscosity in fluid-immersed amorphous materials. We then demonstrate this relationship and its rheological consequences in simulations of stress relaxation in strained filament networks and dense suspensions.

CPP 42: Battery Materials (joint session KFM/CPP)

Chair: Prof. Dr. Anna Grünebohm (Ruhr-University Bochum)

Time: Thursday 9:00–12:35 Location: POT 51

CPP 42.1 Thu 9:00 POT 51

Materialanalyse von NMC111 Kathodenmaterial aus recycelten Lithium-Ionen-Batterien mittels XRD, AFM und EDX/REM — •Claudia Schöberl, Hanno Käss und Stephan Appel — Hochschule Esslingen, Kanalstraße 33, 73728 Esslingen, Deutschland

In einem industriellen Recyclingverfahren für Lithium-Ionen-Batterien wird Kathodenmaterial von der Trägerfolie mit Wasser abgestrahlt und getrocknet. In einem an der Hochschule Esslingen laufenden Forschungsprojekt wird die so gewonnene Schwarzmasse, die hauptsächlich aus NMC111 besteht, mittels Röntgendiffraktometrie (XRD), Rasterelektronenmikroskopie (REM) und elementanalytischen Methoden untersucht, um Hinweise auf die chemische Zusammensetzung und auf strukturelle Veränderungen zu erhalten. Ziel ist es unter anderem, passende Auswahlkriterien für die Qualität des Recyclingmaterials zu definieren, das nach Verarbeitung erneut in Lithium-Ionen-Batterien eingesetzt werden soll. Dazu zählen, neben dem Rest-Bindemittelgehalt, der Kohlenstoffanteil sowie der Anteil an Fremdelementen wie Kupfer und Aluminium. Das wiedergewonnene, recycelte Aktivmaterial wird bei einem Projektpartner zur Herstellung neuer Kathodenfolien verwendet, die in einer Messzelle elektrisch charakterisiert werden. Mittels Rasterkraftmikroskopie (AFM) werden diese neu präparierten Kathodenfolien an der Hochschule Esslingen untersucht. Mit Hilfe eines speziellen Messmodus, der quantitativen nanoskaligen mechanischen Charakterisierung, wird insbesondere die Korrelation von Strukturmerkmalen und mechanischen Eigenschaften überprüft.

CPP 42.2 Thu 9:20 POT 51

Structural response in NCA-type battery cathodes — •Tobias Hölderle[1,2], Peter Müller-Buschbaum[1,2], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]MLZ, TUM, Garching, Germany

Battery-powered electric drivetrains in electric vehicles (EVs) are heavily limited and constrained to the performance of the energy storage device, i.e. battery. Batteries with higher power/energy densities, capacities, and cycling life are needed to increase EVs' performance and reduce greenhouse gas emissions. Mixed high nickel content $Li_xNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA) cathode material is one of a few today that simultaneously possess high energy and power densities at lower costs. However, NCA materials suffer from poor thermal stability and limited power density. They display capacity fading/efficiency loss due to antisite defects (cation mixing) in their structure, actively discussed in literature. In order to address the issue of cation mixing, a systematic ex-situ neutron powder diffraction study was done for a series of electrochemically delithiated NCA cathodes. The collected set of structural data was modeled using full-profile Rietveld method and results were discussed in line with observed electrochemical behavior. It is observed that lithium occupancies showed a decreasing character upon charging, independent from transition metal occupancies and indicating an absence of antisite defects (cation mixing) in the commercial NCA material during cell operation.

CPP 42.3 Thu 9:40 POT 51

Dynamic structure evolution of extensively de-lithiated high voltage spinel LNMO — Nicola Jobst[1], •Neelima Paul[2], Premysl Beran[3,4], Marilena Mancini[1], Ralph Gilles[2], Margret Wohlfahrt-Mehrens[1], and Peter Axmann[1] — [1]Accumulators Materials Research (ECM), ZSW Cen-tre for Solar Energy and Hydrogen Research Baden-Württemberg, DE-89081 Ulm, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, DE-85747 Garching, Germany — [3]Nuclear Physics Institute CAS, CZ-25068 Rez, Czech Republic — [4]European Spallation Source ERIC, Box 176, SE-221 00 Lund, Sweden

High voltage spinel is one of the most promising next-generation cobalt-free cathode materials for Li-ion batteries. Besides the typical compositional range of LixNi0.5Mn1.5O4 0<x<1 in the voltage window 4.90 to 3.00 V, additional 1.5 mol of Li per formula unit can be introduced into the structure, in an extended voltage range to 1.50 V. Theoretically, this leads to significant increase of the specific energy from 690 to 1190 Wh/kg. However, utilization of the extended potential window leads to rapid capacity fading, voltage polarization that lack a comprehensive explanation. In this work, we conducted potentiostatic entropymetry, operando XRD and neutron diffraction on the ordered stoichiometric spinel LixNi0.5Mn1.5O4 within 0 < x < 2.5 in order to understand the dynamic structure evolution and correlate it with the voltage profile. We were able to provide a conclusive explanation for the additional voltage step at 2.10 V, the sloping voltage profile below 1.80 V, and the additional voltage step at ˜3.80 V.

CPP 42.4 Thu 10:00 POT 51

Computational Screening of Oxide Perovskites as Insertion-Type Cathode Material — •Johannes Döhn[1] and Axel Gross[1,2] — [1]Institute of Theoretical Chemistry, Ulm University, Germany — [2]Helmholtz Institute Ulm, Germany

The intermittency of wind and solar power - the solely sustainable energy sources which are considered to be abundantly available - leaves only one consequence: For the transition towards renewable energy systems, efficient and reliable storage technologies are needed. Batteries are one of the most widely used storage devices but current technology based on the transfer of Li-ions faces several challenges including their dependence on critical materials with respect to both, scarcity and toxicity.

In our contribution we will discuss atomic-scale investigations of potential future battery materials carried out using density functional theory (DFT). We employed a high-throughput approach in order to screen the well known material class of oxide perovskites as insertion-type cathode materials and we derived several crucial battery properties including voltage and theoretical energy density for in total 280 compounds. For those candidate materials with promising properties, we evaluated additional features such as the voltage profile and diffusion barriers for ionic transport.

Such in silico investigations significantly narrow down the potential materials space for experimental coworkers and thereby contribute to finding green, cheap and reliable devices for energy storage.

CPP 42.5 Thu 10:20 POT 51

Construction of cobalt oxyhydroxide nanosheets with rich oxygen vacancies as high-performance Lithium-ion Battery anodes — •Yonghuan Fu[1,2], Huaping Zhao[1], Jianhong Liu[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Graphene Composite Research Center, College of Chemistry and Environmental Engineering, Shenzhen University, Shenzhen, P. R. China

Cobalt oxyhydroxide (CoOOH) is a promising anode material for lithium-ion batteries (LIBs) due to its high electronic conductivity and theoretical specific capacity. Herein, CoOOH nanosheets are successfully obtained using a facile one-pot method, and a hierarchical nanoporous structure is formed by oxidizing cobalt hydroxide (Co(OH)2) in NaOH and (NH4)2S2O8 solution. The CoOOH anode shows better electrochemical performance compared to Co(OH)2 and Co3O4 electrodes when applied to LIBs. The hierarchical nanoporous structure and high electronic conductivity of the CoOOH anode contribute to its outstanding initial discharge capacity, high initial coulombic efficiency, and excellent cyclability. Experiments and density functional theory (DFT) calculations confirmed that the high ICE and prominent rate capability of the nanosheets could be ascribed to the rapid and complete conversion reaction of CoOOH upon lithiation/delithiation facilitated by hydroxyl groups and oxygen vacancies. This study provides new insights into the structure-property relationship of transition-metal oxyhydroxide anode materials for LIBs.

CPP 42.6 Thu 10:40 POT 51

The dielectric behaviour of lithium intercalated graphite anodes - as a function of the state of charge — •Simon Annies, Chiara Panosetti, and Christoph Scheurer — Fritz Haber Institut Berlin

The dielectric behaviour of battery materials is a crucial piece of information for understanding atomistic mechanics and modelling diffusion-and charging processes. However, for the most common anode material in today's lithium ion batteries (lithium intercalated graphite), literature results regarding this property are sparse, conflicting and only available for graphite, i.e. the empty state of charge (SOC).

Utilizing our recently developed DFTB parametrization [1] which is based on a machine-learned repulsive potential, we are – for the first time – able to compute the dielectric behaviour of lithium intercalated graphite for the entire range of charge from 0% to 100% - finding a linear dependency from around ϵ_r=7 at 0% SOC to around 25 at 100% SOC. We achieve this by sampling the Coulomb interactions between pairs of Li-ions and vacancies in large cells with varying intercalant concentrations in the adjacent layers.

Our results agree with experiments in the limit of "empty" graphite, as well as for (bilayer-) graphene, which we consider a validation of our approach. With this, we lay an important piece of foundation for the understanding and multi-scale modelling of entire charging and discharging cycles of graphite anodes in Li-ion batteries.

[1] Anniés, Simon, et al., Materials 14.21 (2021): 6633.

CPP 42.7 Thu 11:00 POT 51

Hypothetical t-LGPO as a good ionic conductor, and the influence of Li core electrons on diffusion — Giuliana Materzanini[1], •Nicola Marzari[2,3], and Gian-Marco Rignanese[1] — [1]Modelling Division, Universite catholique de Louvain, 1348 Louvain-la-Neuve, Belgium — [2]Theory and Simulations of Materials (THEOS), Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland — [3]National Centre for Computational Design and Discovery of Novel Materials (MARVEL), Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland

Following the computationally found high Li-ion conductivity in tetragonal Li10GeP2O12 (t-LGPO), we study here the role of Li core electrons on Li diffusion in this hypothetical superionic material. We calculate Li diffusivity from two sets of Car-Parrinello canonical molecular dynamics simulations, one using Li pseudopotential with all electrons (1s22s1), and one with just one electron (2s1). The Arrhenius plots show a marked influence of the Li 1s electrons on the Li-ion diffusivity in t-LGPO, being the diffusion coefficient at 600 K one order of magnitude larger, and the activation barrier between 600 and 1200 K 1.5 times smaller, for the Li all-electrons with respect to the Li one-electron calculations. Similar sets of simulations performed for the analogue sulfide material, tetragonal Li10GeP2S12 (LGPS), show, oppositely, that for LGPS the influence of Li 1s electrons on Li diffusivity is minimal. The different response of Li mobility to the explicit treatment of 1s electrons reveals fundamental differences in the ionic conductivity mechanism in these two classes of materials.

15 min. break

CPP 42.8 Thu 11:35 POT 51

Sodiation-induced reactivation of micro-nano flower for ultralong cycling life sodium-ion batteries — •Yulian Dong, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

A rational micro-nano hierarchical structure is demonstrated to prolong the cycle life of sodium-ion batteries (SIBs) by relieving the volume expansion and preventing active material agglomeration. In this work, micro-nano flower 3D-VSx was fabricated as an anode electrode for SIBs. The advanced features of micro-nano flower and the unique crystal structures of NiAs-type vanadium sulfides synergistically contribute to enhancing the electrochemical kinetics of 3D-VSx, and finally achieved remarking electrochemical performances with an ultra-high capacity (961.4 mAh/g at 2 A/g) and an ultra-long cyclability (more than 1500 cycles). Furthermore, ex situ X-ray diffraction, Raman, and SEM bring to light a gradual reactivation process of 3D-VSx for sodium storage. Fortunately, upon reactivation, the electrochemical impedance of the 3D-VSx anode gradually weakens, and the diffusion-controlled charge storage mode further dominates compared to the capacitively-controlled mode, all of which facilitate the 3D-VSx to maintain a stable sodium storage capability. This work presents a general approach for preparing super-high specific capacity and rate capacity electrode materials for further improving the SIBs performance.

CPP 42.9 Thu 11:55 POT 51

Sodium diffusion mechanism in NASICON solid electrolyte materials studied via quasi-elastic neutron scattering — •Ivana Pivarníková[1,2], Stefan Seidlmayer[1], Martin Finsterbusch[3], Gerald Dück[3], Niina Jalarvo[4], Peter Müller-Buschbaum[1,2], and Ralph Gilles[1] — [1]TUM, MLZ, Garching, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [3]FZJ, IEK-1, Jülich, Germany — [4]ORNL, Oak Ridge, TN, USA

The sodium superionic conductor materials, also known as NASICON, have been a widely studied class of solid electrolytes for Na-ion based all-solid-state batteries. The aim of this work is to clarify the reason for extremely high conductivity exhibited by Na1+xZr2SixP3-xO12 (0-x-3) and to explain the role of the monoclinic to rhombohedral phase transition for the material with x=2.4, which supposedly occurs at around 170°C. We also investigate the overall temperature dependence of the ionic conductivity in the temperature range of 297-640K. The quasi-elastic neutron scattering (QENS) is used to measure the spatial and temporal dynamic properties of diffusion of Na-ions in the crystal structure. The Na-ion diffusion mechanism can be described by the right choice of the diffusion model. Important parameters, such as diffusion coefficients, activation energies, jump distances between the occupation sites and residence times are extracted from the measured and modelled QENS data. Temperature dependent X-ray diffraction data have been obtained and analysed in order to confirm the results obtained from the QENS data.

CPP 42.10 Thu 12:15 POT 51

3D flower-like MnV12O31 center dot 10H2O as a high-capacity and long-lifespan cathode material for aqueous zinc-ion batteries — •Yan Ran[1], Yude Wang[2], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Yunnan Key Laboratory of Carbon Neutrality and Green Low-carbon Technologies, Yunnan University, 650091 Kunming, China

In this work, MnV12O31 center dot 10H2O (MnVO) synthesized via one-step hydrothermal method is proposed as a promising cathode material for AZIBs. Because its stable layered structure and hieratical morphology provide a large layer space for rapid ion transports, this material exhibits a high specific capacity (433 mAh g-1 at 0.1 A g-1), outstanding long-term cyclability (5000 cycles at current density of 3 A g-1), and sufficient energy density (454.65 Wh kg-1). To illustrate the intercalation mechanism, ex-situ X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and X-ray photoelectron spectroscopy (XPS) are adopted, uncovering a H+/Zn2+ dual-cation co-intercalation processes. Besides, density functional theory (DFT) calculation analysis shows that MnVO has a delocalized electron cloud and the diffusion energy barrier of Zn2+ in MnVO is low, which promotes the Zn2+ transport and, consequently, improves the reversibility of the battery upon deep cycling. The results provide key and enlightening insights for the design of high-performance vanadium-oxide-based cathode materials for AZIBs.

CPP 43: Organic Electronics and Photovoltaics III (joint session CPP/HL)

Time: Thursday 9:30–12:30 Location: GÖR 226

CPP 43.1 Thu 9:30 GÖR 226

Determining exciton diffusion lengths in organic non-fullerene acceptors with Kinetic Monte Carlo Simulation — •Wenchao Yang, Safakath Karuthedath, Catherine Castro, Julien Gorenflot, and Frederic Laquai — KAUST Solar Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Optimal exciton diffusion length (L_D) is a key parameter for reducing losses during exciton to charge carrier conversion in organic solar cells (OSC). However, different research groups report contradicting numbers for the same non-fullerene acceptors (NFA) using different lifetimes to calculate L_D. In this work, in order to verify the measured L_D's in NFAs (ITIC, IT4F, ITM and IT2Cl) using transient absorption (TA) spectroscopy, we employed the Kinetic Monte Carlo (KMC) method to simulate the exciton dynamics and calculate the corresponding L_D. With the assumption of Förster resonant energy transfer type exciton hopping rate in a cubic lattice, the TA decay kinetics under different fluences are reproduced by the KMC simulation, and the only free parameter: the energetic disorder σ is extracted. The use of the lifetime τ measured by time-resolved photoluminescence in neat NFA enables to reproduce the transients using more realistic σ values. The L_D's in the NFAs are further calculated with the τ's and found to be consistent with the experimental values. This work provides microscopic descriptions of exciton diffusion and more insight into the determination of L_D in organic semiconductors.

CPP 43.2 Thu 9:45 GÖR 226

A thorough analysis of conformational locking and related electrical properties in fluorinated thieno-quinoxalines — •Md Moidul Islam[1,2], Arthur Markus Anton[1,2,5], Shahidul Alam[6], Rico Meitzner[1,2], Christos L. Chochos[3,4], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC),Friedrich Schiller University Jena, Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Jena, Germany — [3]Institute of Chemical Biology, National Hellenic Research Foundation, Athens 11635, Greece — [4]Advent Technologies SA, Patra, Greece — [5]Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Leipzig, Germany — [6]King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Physical Sciences and Engineering Division (PSE), Material Science and Engineering Program (MSE), Kingdom of Saudi Arabia

Thieno-quinoxaline derivatives with low band gaps are promising donor materials for organic solar cells. Therefore, investigations have been conducted on thieno-quinoxaline polymers with systematically varied fluorination sites. Cyclic voltammetry revealed that fluorination lowers both the HOMO as well as LUMO energy levels, whereas the size of photochromic units is affected through the particular kind of fluorination demonstrated by UV-Vis absorption spectra. Furthermore, excitation-emission mapping exposed excitation-independent and excitation-selective PL pathways.

CPP 43.3 Thu 10:00 GÖR 226

Orientation and Order of Molecular Subunits and Excited State Dynamics in a P3HT Bottlebrush Copolymer — •Arthur Markus Anton[1,2], Friedrich Kremer[1], Jenny Clark[2], and Frank Cichos[1] — [1]Leipzig University, Peter Debye Institute for Soft Matter Physics, Linnéstr. 5, 04103 Leipzig, Germany — [2]The University of Sheffield, Department of Physics and Astronomy, Hounsfield Rd, Sheffield S37RH, United Kingdom

Orientation and order at different length scales are believed to play a crucial role for the performance of organic semiconductor devices. Taking advantage of the material properties of *bottlebrush copolymers* and gain control of structure formation, a poly-(3-hexylthiophene) grafted copolymer has been studied [1]. In order to investigate the structure on the molecular scale the technique of *Infrared Transition Moment Orientational Analysis* (IR-TMOA) has been employed [2,3]. The absorbance of structure-related bands is evaluated depending on the inclination of the sample film (ϑ) and polarization of the IR light (φ). This combination then allows to determine the tensor of absorption separately for the respective molecular moieties and to deduce their orientation (Θ,Φ) relative to a sample-fixed coordinate system. In addition *transient absorption* measurements have been conducted. The dynamics of exciton and polaron formation and decay has been investigated and the derived results on the basis of the bottlebrush copolymer are compared with results from linear P3HT. [1] Heinrich and Thelakkat, *J. Mater. Chem. C* **4** (2016) 5370 [2] Anton et al, *J. Am. Chem .Soc.* **137** (2015), 6434 [3] Anton et al, *Macromolecules* **49** (2016) 1798

CPP 43.4 Thu 10:15 GÖR 226

Utilizing High Gain and Spectral Narrowing for Near-Infrared Organic Photodetectors — •Louis Conrad Winkler[1], Jonas Kublitski[2], Johannes Benduhn[1], and Karl Leo[1] — [1]TU Dresden, Germany — [2]Federal University of Technology Paraná UTFPR, Curitiba, Brazil

There is a multitude of applications for infrared photodetectors that demand high-volume fabrication, including blood oxygen determination, continued monitoring of food quality, control of industrial processes, and many more. Organic photodetectors (OPDs) have great potential to enrich today*s photodetector marked with their low-cost fabrication, flexible devices and tunable response. However, most studied organic semiconducting materials have neglectable absorption above 1000 nm. This contribution presents a donor-acceptor blend with a low-energy and broad charge-transfer (CT) feature. To overcome the inherent increase of charge carrier recombination of such low-energy systems, we introduce two photocurrent multiplication (PM) mechanisms. By embedding this OPD into an optical micro-cavity, a spectral response (SR) of 15 AW-1 at 1095 nm is achieved. Furthermore, a very narrow response of only 18 nm makes this architecture ideal for spectroscopic resolved measurements that could be easily integrated into CMOS readout circuitry due to the optimization for operation under reverse bias.

CPP 43.5 Thu 10:30 GÖR 226

Realizing a high-performance, fully thermal-evaporated, blue narrowband organic photodetector — •Tianyi Zhang, Johannes Benduhn, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Dresden, Germany

Organic photodetector (OPD) boasts of its tunable absorption window, mechanical flexibility, transparency, non-toxicity, facile processing, and cheaper cost. Recent development of high-performing polymers and small molecules further reveals its potential in numerous communication and biomedical applications. To realize visible light communication, commercially available inorganic photodetector usually incorporates additional optical filters, which further increases the complexity and cost of the sensing system. Therein, we demonstrate a blue absorbing organic photodetector with ultrahigh specific detectivity (D^*) approaching 10^{14} Jones. By employing a wide bandgap hole transporting layer BF-DPB with Rubrene:C_{60} active layer, the absorption peaks at 450nm with an external quantum efficiency (EQE) of 50% at zero bias. The parasitic absorption renders the narrowband characteristic of the blends to span merely over the blue wavelength region. Upon BF-DPB incorporation, ultrafast responses are also observed at sub-microseconds. We conclude that the judicious choice of transporting layer is critical for achieving application-tailored properties, namely high speed or high D^*. To date, those values are among the best-reported blue OPDs.

CPP 43.6 Thu 10:45 GÖR 226

Investigation of high performance organic photodetectors based on single component photoactive layer — •Jakob Wolansky[1], Cedric Hoffmann[2], Felix Talnack[3], Michel Panhans[4], Donato Spoltore[5], Stefan C.B. Mannsfeld[3], Frank Ortmann[4], Natalie Banerji[2], Johannes Benduhn[1], and Karl Leo[1] — [1]IAPP, TU Dresden — [2]University of Bern — [3]Cfaed, TU Dresden — [4]TU Munich — [5]University of Parma

In organic semiconductor applications such as organic photovoltaics and photodetectors, an intermolecular interface with an energetic gradient between electron donating and accepting materials is usually required for efficiently generating charges. This driving force facilitates the dissociation of the photogenerated excitons. At the same time, this energy offset reduces the maximum possible open-circuit voltage, and the additional interface can act as a recombination site and increases the dark current. Therefore, single-component devices are extensively researched to overcome these drawbacks.

Here, we report on single-component devices that perform very well as organic photodetectors. By utilizing different device processing parameters and employing different interface layers, we optimized the device characteristics such as external quantum efficiency, dark current, and specific detectivities of more than 1e13 Jones. Investigations of the morphology, combined with ultrafast transient absorption measurements, give insight into the charge generation mechanism in our material system.

CPP 43.7 Thu 11:00 GÖR 226

Reduced defect density in crystalline halide perovskite films via methylamine treatment for the application in photodetectors — •Emilia Rosa Schütz[1], Azhar Fakharuddin[1], Yenal Yalcinkaya[2,3], Efrain Ochoa-Martinez[4], Shanti Bijani[5], Abd. Rashid bin Mohd Yusoff[6], Maria Vasilopoulou[7], Tobias Seewald[1], Ullrich Steiner[4], Stefan Weber[2,3], and Lukas Schmidt-Mende[1] — [1]University of Konstanz, Konstanz, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany — [3]Johannes Gutenberg University Mainz, Mainz, Germany — [4]Adolphe Merkle Institute, University of Fribourg, Fribourg, Switzerland — [5]Unidad de Nanotecnología, Centro de Supercomputador y Bioinnovación SCBI, Universidad de Málaga, Málaga, Spain — [6]Pohang University of Science and Technology, Pohang, Republic of Korea — [7]National Center for Scientific Research Demokritos, Attica, Greece

The quality of a perovskite layer strongly depends on the processing conditions. Consequently, the fabrication process is often complex, and reproducibility is a challenge. Our methylamine gas-based method is able to recrystallize perovskite layers of any given quality in a controlled way, leading to millimeter-sized domains. Crystallinity significantly increases upon methylamine treatment, and crystal growth follows a preferred orientation. Photoluminescence- and space-charge limited current measurements imply that the trap density decreases after recrystallization. When applied in photodetectors, the improved film quality of the recrystallized films leads to increased detectivities and shorter response times.

15 min. break

CPP 43.8 Thu 11:30 GÖR 226

Reducing Dark Current in Highly Ordered Rubrene:C_{60} Heterojunctions for Organic Photodetectors — •Anna-Lena Hofmann[1], Jakob Wolansky[1], Lucy Winkler[1], Max Herzog[1], Felix Talnack[2], Eva Bittrich[3], Johannes Benduhn[1], and Karl Leo[1] — [1]IAPP, TU Dresden, Dresden, Germany — [2]Cfaed, Dresden, Germany — [3]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

Vacuum-deposited rubrene can form highly ordered phases, demonstrating an exceptionally high charge carrier mobility for holes ($> 10\,\mathrm{cm^2\,V^{-1}\,s^{-1}}$) even in thin films. Depending on the post-treatment of our films, we can control different crystalline phases. For fast-response OPDs, the triclinic phase is very promising since it exhibits high hole mobility in the vertical direction. However, the high surface roughness is a key reason why these devices fall short in specific detectivity. In this work, we employ different strategies to reduce the impact of Ohmic shunts within the device to minimize the noise current of our devices. We characterize the morphology of our films and investigate the performance parameters of fully working devices. Finally, these characteristics are compared to rubrene's other two crystalline phases.

CPP 43.9 Thu 11:45 GÖR 226

Utilizing charge-transfer states for narrowband and highly sensitive photodetection — •Johannes Benduhn, Louis Conrad Winkler, Awais Sawar, Jonas Kublitski, and Karl Leo — IAPP, TU Dresden, Germany

Near-infrared (NIR) spectroscopic material sensing has the potential to revolutionize many aspects of life, ranging from food control to material determination. However, currently available products are either too bulky or too expensive to be used in mobile customer applications. In this regard, organic photodetectors (ODPs) can open new perspectives due their cheap and versatile processing techniques. Nevertheless, the external quantum efficiency (EQE) as well as the specific detectivity of those devices in the NIR wavelength range are still lacking behind. In this contribution, we explore photomultiplication (PM) in fully vacuum deposited OPDs. Broadband devices achieve a maximum EQE of almost 2000 % at -10 V. Employing very sensitive measurement techniques as well as optical modelling of our devices, we are able to proof that the photomultiplication can take place even if weakly absorbing charge-transfer states are responsible for the photon harvesting. Employing a suitable donor-acceptor system as well as an optimized device architecture for photomultiplication and constructive interference in the NIR wavelength range, we achieve narrowband OPDs with the spectral response of more than $10\,\mathrm{A\,W^{-1}}$ at a wavelength of 1100 nm with full width at half maximum even below 20 nm. These results demonstrate the versatility of OPDs and their potential for spectroscopic material sensing.

CPP 43.10 Thu 12:00 GÖR 226

Design of Integrated All-Organic Oxygen Sensors — •Toni Bärschneider and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden

Organic electronic devices, such as light-emitting diodes (OLEDs) and photodetectors (OPDs), are ideal for sensor applications because of their versatility and flexibility. Additionally, they can be easily fabricated on any substrate, making integrated sensor applications possible. This allows for easy miniaturization and cheap fabrication. Organic room temperature phosphorescence (RTP) materials are well suited for optical oxygen sensing because of their strong oxygen dependency.

In this work, we developed a monolithic all-organic oxygen sensor composed of a RTP sensing layer, an ultraviolet OLED as an excitation source, and a narrow bandwidth OPD for detection. The RTP sensing layer simultaneously shows fluorescence and phosphorescence at room temperature, which enables self-referencing to avoid photodegradation-caused distortion. Due to the long phosphorescence lifetime, sensing within the ultra-trace range is possible.

The presented sensors overcome drawbacks of current optical oxygen sensors, such as complexity, expensive read-out electronics, and a lack of possible miniaturization.

CPP 43.11 Thu 12:15 GÖR 226

Atomistic insights on the electrode material CuDEPP — •Christoph Jung[1,2] and Timo Jacob[1,2] — [1]Universität Ulm, Institut für Elektrochemie, Ulm, Germany — [2]HIU, Ulm, Germany

Devices for electrical energy storage need to provide high energy yields as well as output power while at the same time guaranteeing safety, low costs and long operation times. The porphyrin CuDEPP [5,15-bis(ethynyl)-10,20-diphenylporphinato]copper(II) is a promising electrode material for various battery systems both as anode or cathode. CuDEPP combines the positive properties of lithium ion batteries (high energy density) with those of a supercapacitor (fast electron release and absorption). While its functionality has been demonstrated experimentally, there had been no atomistic information as to why CuDEPP expresses these interesting properties or how the incorporation of ions affects its structure. Starting with the smallest possible unit (i.e. a single molecule) we successively increased the spatial dimensionality of the structure by studying: a) di- and trimers, b) molecular stacking in a 1D chain, c) extending these chains to planar CuDEPP sheets and finally c) a three-dimensional extended polymer structure. Combining the individual results of the molecule, the chain, the plane and the extended polymer lead to a comprehensive and consecutive understanding of the CuDEPP system. Afterwards the insertion (or intercalation) of different ions (including Li, Mg and Na) has been studied. Based on the optimal ion intercalation structure, discharge voltage curves have been calculated and compared to experimental measurements.

CPP 44: Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)

Time: Thursday 9:30–13:00 Location: MER 02

CPP 44.1 Thu 9:30 MER 02

Dynamic wetting of concentrated granular suspensions — •Reza Azizmalayeri, Peyman Rostami, and Günter K. Auernhammer — Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

Concentrated granular suspensions are employed in a variety of processes where the contact line dynamics and internal structure of the suspension interact. The process can be characterized using individual particle analysis and average suspension descriptions. Along the contact line, particles interact with each other and the substrate, and the shear rate influence the suspension's non-Newtonian rheological behavior. In this study, we use fluorescently-labeled tracer particles in a refractive index-matched silica suspension. We track the motion of the tracer particles in the concentrated suspension with astigmatism particle tracking velocimetry (APTV). Averaging over single tracks gives the flow profile in a droplet near the advancing contact line. In addition, side-view allows characterizing the drop shape. The behavior of high-concentration suspensions near contact lines differs significantly from that of simple liquids. Near the advancing contact line, we observe the fast-moving layering of suspensions close to the substrate, which is controlled by the suspension's rheology. Near the receding contact line, the suspension adheres to its previous layer and moves on top of it. Initially, there is an unsteady motion, which becomes stationary with time.

CPP 44.2 Thu 9:45 MER 02

Sliding drops: towards a universal law of friction — Xiaomei Li[1], Francisco Bodziony[2], Mariana Yin[2], Holger Marshall[2], Rüdiger Berger[1], and •Hans-Jürgen Butt[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz — [2]Computational Multiphase Flows, Technische Universität Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt

Liquid drops moving on tilted surfaces are an everyday phenomenon and are important for many industrial applications. Still, it is not possible to predict their velocity. To make a step forward in quantitative understanding, we measured the velocity U, width w, length, advancing Θ_a, and receding contact angle Θ_r of liquid drops sliding down inclined flat surfaces. By solving the equation of motion, we determined the friction force versus slide velocity for different hydrophobic surfaces. The friction force acting on moving drops of polar and non-polar liquids with viscosities ranging from 10^{-3} to 1 Pa s can empirically be described by $F_f(U) = F_0 + \mu w Ca^\alpha$ for the whole relevant velocity range. Here, $Ca = U\eta/\gamma$ is the capillary number, in which η is the viscosity and γ the surface tension of the liquid. The friction coefficient μ is in the range of 1 - 3 N/m for all liquid/surface combinations. For viscosities above 0.006 Pa s, we find $\alpha = 1.0$. Bulk and wedge viscous dissipation can fully account for the velocity-dependent friction force. These results were confirmed by direct numerical diffuse-interface simulations of the flow pattern inside sliding drops. We demonstrate that the Furmidge-Kawasaki equation, is also valid in the dynamic case.

CPP 44.3 Thu 10:00 MER 02

Spreading of soft elasto-viscoplastic droplets — •Maziyar Jalaal[1], Cassio Oishi[1], and Hugo França[1,2] — [1]Institute of Physics, University of Amsterdam, Amsterdam, The Netherlands — [2]Sao Paulo State University, Sao Paulo, Brazil

The spreading under surface tension of a droplet of complex fluid with elastic and plastic properties is studied. Unlike Newtonian fluids, the droplet converges to a final equilibrium shape once the driving stresses inside the droplet fall below the critical yield stress. Scaling laws are presented for the final radius and complemented with an asymptotic analysis for shallow droplets. Moreover, numerical simulations using the volume-of-fluid method and an elastoviscoplastic (EVP) constitutive law, and experiments with an aqueous solution of Carbopol, are presented.

CPP 44.4 Thu 10:15 MER 02

Stick-slip Contact Line Dynamics in Forced Wetting of Polymer Brushes — •Daniel Greve[1], Simon Hartmann[1], and Uwe Thiele[1,2] — [1]Institut für Theoretische Physik, WWU Münster — [2]Center for Nonlinear Science (CeNoS), WWU Münster

We study the wetting of adaptive substrates using a mesoscopic hydrodynamic model for a liquid droplet on a polymer brush, refining the model in [1]. First, we show that Young's law still holds for the macroscopic equilibrium contact angle and that on the mesoscale a Neumann-type law governs the shape of the wetting ridge (comparable to the case of elastic substrates [2]). Further, we numerically examine the wetting ridge dynamics for a moving meniscus, i.e., we consider an "inverse Landau-Levich geometry" where a brush-covered plate is introduced into a bath. We find stick-slip motion in good qualitative agreement with experimental observations [3,4] and discuss criteria for the onset of the corresponding instability.

[1] U. Thiele and S. Hartmann, *Eur. Phys. J.-Spec. Top.*, 2020, 229, 1819-1832.
[2] B. Andreotti and J. H. Snoeijer, *Annu. Rev. Fluid Mech.*, 2020, 52, 285-308.
[3] S. Schubotz et al., *Adv. Colloid Interface Sci.*, 2021, 294, 102442.
[4] L. Wan, X. Meng, Y. Yang, J. Tian and Z. Xu,*Sci. China Chem.*, 2010, 53, 183-189.

CPP 44.5 Thu 10:30 MER 02

Demixing of liquid PDMS during dewetting into the equilibrium state — •Khalil Remini[1], Leonie Schmeller[2], Dirk Peschka[2], Barbara Wagner[2], and Ralf Seemann[1] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Weierstrass-Institute, Berlin University, Berlin, Germany

The study of micrometer-sized equilibrium droplets on elastic substrates is of great interest because, due to negligible gravity, other interactions such as elastic or capillary forces and their mutual influence can easily be investigated, so deviations from the expected behaviour at larger scales becomes visible. This applies in particular to soft solids like PDMS that are typically considered as ideal rubbers on the macro scale. Our experimental system is composed of liquid polystyrene (PS) droplets on a viscoelastic substrate consisting of cross-linked polydimethylsiloxane (PDMS) of different elasticities. Using atomic force microscopy (AFM), we analyse the topography of the materials and thus their contact angles with high precision, we also use AFM to demonstrate the existence of non-cross-linked liquid PDMS that migrates from the elastic PDMS toward the three-phase contact line TPCL to form a demixed liquid ring around the dewetted PS droplet. In that situation, on the nanometer distance around the TPCL, liquid PS meets liquid PDMS instead of being in direct contact with the soft solid PDMS. Further analysis allows us to say that this phenomenon also exists during the dewetting of liquid polystyrene in the same type of elastic solids.

CPP 44.6 Thu 10:45 MER 02

How droplets dry on stretched soft substrates — •Binyu Zhao, Yixuan Du, and Günter K. Auernhammer — Leibniz Institute of Polymer Research Dresden, Dresden 01069, Germany

Droplets evaporation on solid substrates is a ubiquitous phenomenon and relevant in many natural and industrial processes. Well known are the coffee-ring. Many studies have succeeded in promoting, suppressing or even reversing the formation of coffee-ring by using non-spherical particles, surfactants, patterned substrates, and so on.

Here, we show that a uniaxial stretching of soft substrates strongly controls the dynamics of droplet evaporation and particle deposition through controlling the contact line motion. Water droplet evaporates with an elongated non-circular contact line on the stretched substrates and switches the elongation direction during evaporation. The contact line evolution depends on the orientation of the contact line relative to the stretching direction. When nanoparticles are added into the liquid, the circular deposition pattern, i.e., the so-called coffee-ring, becomes elongated along the direction perpendicular to the stretching direction. Particularly, such non-circular deposition pattern exhibits periodic height gradients along its rim. The finer structure of the pattern can be controlled by applying different stretching ratios to the soft substrate and thus are correlated to the anisotropic surface stresses near the contact line. The findings broaden our understanding of droplet wetting and evaporation on soft and anisotropic substrates, and open the way to reshaping the coffee-ring to allow anisotropic, non-circular patterning.

CPP 44.7 Thu 11:00 MER 02

Gradient dynamics model for sessile drop evaporation in a gap: from simple to applied scenarios — •Simon Hartmann[1], Uwe Thiele[1], Christian Diddens[2], and Maziyar Jalaal[3] — [1]Institut für Theoretische Physik and Center for Nonlinear Science, Universität Münster — [2]Physics of Fluids group, Max Planck Center Twente for Complex Fluid Dynamics, and J. M. Burgers Center for Fluid Dynamics, University of Twente — [3]Van der Waals-Zeeman Institute, Institute of Physics, University of Amsterdam

We consider an evaporating drop of volatile partially wetting liquid on a rigid solid substrate. In addition, the setup is covered with a plate, forming a narrow gap with the substrate. First, we develop an efficient mesoscopic description of the liquid and vapor dynamics in a gradient dynamics form. It couples the diffusive dynamics of the vertically averaged vapour density in the narrow gap to an evolution equation for the drop profile. The dynamics is purely driven by a free energy functional that incorporates wetting, bulk and interface energies of the liquid as well as vapour entropy.

Subsequently, we employ numerical simulations to validate the model against both experiments and simulations based on Stokes equation. Finally, we show that the gradient dynamics approach allows for extensions of our model to cover more intricate scenarios, e.g., spreading drops of volatile liquid on polymer brushes or on porous media.

15 min. break

CPP 44.8 Thu 11:30 MER 02

Modeling the temporal evolution and stability of thin evaporating films for wafer surface processing — •Max Huber[1,2,3], Xiao Hu[1,2,3], Andreas Zienert[1,2,3], and Jörg Schuster[1,2,3] — [1]Fraunhofer Institute for Electronic Nano Systems ENAS, Technologie-Campus 3, 09126 Chemnitz, Germany — [2]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Rosenbergstr. 6, 09126 Chemnitz, Germany — [3]Center for Microtechnologies, Chemnitz University of Technology, Reichenhainer Str. 70, 09126 Chemnitz, Germany

Thin liquid films play a crucial role for many applications, e.g., coating, particle deposition, wafer bonding, and the cooling of electronic devices. As an example, we investigate the evaporation of thin water films on $LiTaO_3$. *Ab initio* density functional theory is used to calculate the Gibbs free energy of adsorption. These results are fitted to an expression of the Gibbs free energy which is derived from the disjoining pressure, consisting of molecular and structural components. In this way, the parameters for the disjoining pressure can be determined. A combination of literature-known models for spin drying and evaporation is used to analyze the temporal evolution of the water layer. The vapor above the water layer is modeled by diffusion and a mass balance is applied at the water-air interface. The results can be used to optimize the process time needed to reach the equilibrium thickness of the water layer. In addition, computational fluid dynamics simulations are utilized to investigate the evaporation in a wafer bond chamber during pump-down.

CPP 44.9 Thu 11:45 MER 02

Electrokinetic, electrochemical and electrostatic surface potentials of the pristine water liquid-vapor interface — •Maximilian R Becker and Roland R Netz — Freie Universität Berlin, Berlin, Germany

Although conceptually simple, the interface between liquid water and vapor displays rich behavior and is subject to intense experimental and theoretical investigations. Different definitions of the electrostatic surface potential as well as different calculation methods, each relevant for distinct experimental scenarios, lead to widely varying potential magnitudes. Here, based on density-functional-theory (DFT) molecular dynamics (MD) simulations, different surface potentials are evaluated and compared to force-field (FF) MD simulations. The laterally averaged electrostatic surface potential, accessible to electron holography, is dominated by the trace of the water molecular quadrupole moment and therefore differs strongly between DFT and FF MD. Thus, when predicting electrostatic potentials within water molecules DFT simulation methods need to be used. The electrochemical surface potential inside a neutral atom, relevant for ion transfer reactions and ion surface adsorption, is much smaller and depends specifically on the atom radius. Charge transfer between interfacial water molecules leads to a sizable surface potential as well. However, when probing electrokinetics by explicitly applying a lateral electric field in DFT-MD simulations, the electrokinetic zeta-potential turns out to be negligible. Thus, interfacial polarization charges from charge transfer between water molecules do not lead to a significant electrokinetic mobility.

CPP 44.10 Thu 12:00 MER 02

How Charges Separate at Moving Contact Lines — •Aaron D. Ratschow[1], Lisa S. Bauer[1], Pravash Bista[2], Stefan A. L. Weber[2,3], Hans-Jürgen Butt[2], and Steffen Hardt[1] — [1]Technische Universität Darmstadt, Darmstadt, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany — [3]Johannes Gutenberg Universtität, Mainz, Germany

Spontaneous charge accumulation in sliding drops is ubiquitous in nature and has been the subject of research activities for over two decades. Despite the growing number of experimental investigations in recent years, the physical mechanism behind the charging remains poorly understood. We identify the origin of charge separation as the dewetting of the immobilized part of the electric double layer (EDL) by the moving contact line. This layer of physically or chemically bound surface charges depends strongly on the local EDL structure, which is disturbed by the vicinity of the gas-liquid interface and the flow in the liquid. We summarize the physics of charge separation in an analytical model that predicts parametric dependencies on surface chemistry, wetting, and liquid properties. The results agree well with our experiments and numerical simulations and uncover decreasing charge separation with decreasing dynamic contact angle and increasing contact line velocity. Our findings reveal the universal mechanism of charge separation at moving contact lines, not limited to drops, with broad implications for the field of wetting.

CPP 44.11 Thu 12:15 MER 02

Beyond the plate capacitor: Calculating the full dielectric tensor for arbitrary system geometries — •David Egger, Christoph Scheurer, and Karsten Reuter — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Realistic models for catalytic reactions at aqueous interfaces require a profound understanding of the electrostatic properties in the vicinity of the solvated catalytic complex, in particular for (photo-)electrochemical reactions with charged intermediates. However, explicit quantum mechanical simulations of these systems on the required length- and time-scales remain oftentimes out of reach. Coarse-graining the electrostatic response of the molecular solvent into a continuum dielectric, described by the dielectric permittivity tensor $\boldsymbol{\varepsilon}$, can hence be a necessity. Existing coarse-graining protocols for $\boldsymbol{\varepsilon}$ typically assume a separation of the dielectric response parallel and perpendicular to the active interface. This approximation is equivalent to two decoupled sets of in-series plate capacitors and ignores potential nonzero off-diagonal elements in the $\boldsymbol{\varepsilon}$ tensor.

In this contribution, we present a comprehensive and general formalism to coarse-grain molecular solvents into a truly anisotropic $\boldsymbol{\varepsilon}$ beyond this approximation. We obtain the full, spatially resolved dielectric tensor for arbitrary system geometries with no prior assumptions on boundary conditions. Common bulk and slab formulas are obtained as special cases. The approach is applied exemplarily to bulk water, water-dichloroethane liquid-liquid interfaces, and solvated platinum nanoparticles following from Wulff constructions.

CPP 44.12 Thu 12:30 MER 02

Asymmetric Sessile Compound Drops — •Jan Diekmann and Uwe Thiele — Westfälische Wilhelms-Universität, Münster, Germany

We consider compound drops of two immiscible liquids on a rigid solid substrate. Having established a mesoscopic model (amending [1]) consistent with the macroscopic description of [2,3], we show for one-dimensional (1D) substrates that asymmetric compound drops can be energetically favoured using continuation techniques. Furthermore, we investigate selected dewetting and coarsening processes and discuss emerging steady compound drops for two-dimensional (2D) substrates, thereby discussing the relation of 1D and 2D results.

[1] A. Pototsky et al., ”Morphology changes in the evolution of liquid two-layer films”. J. Chem. Phys. 122, 224711, 2005.

[2] L. Mahadevan, M. Adda-Bedia, and Y. Pomeau., ”Four-phase merging in sessile compound drops”. J. Fluid Mech. 451, 411-420, 2002.

[3] M. J. Neeson et al., ”Compound sessile drops”. Soft Matter 8, 11042-11050, 2012.

CPP 44.13 Thu 12:45 MER 02

Steering droplets on substrates with plane-wave wettabil-

ity patterns and deformations — •Josua Grawitter and Holger Stark — Technische Universität Berlin, Institut für Theoretische Physik, Straße des 17. Juni 135, 10623 Berlin

Droplets are set in motion on substrates with a spatio-temporal wettability pattern as generated, for example, on light-switchable surfaces. To study such cases, we implement the boundary-element method to solve the governing Stokes equations for the fluid flow field inside and on the surface of a droplet and supplement it by Cox–Voinov friction for the dynamics of the contact line. One objective of our research is targeted microfluidic transport of such droplets. In earlier work we investigated how a droplet can be steered by imposing a wettability pattern on the substrate [Grawitter and Stark, Soft Matter **17**, 2454 (2021)]. As a next step, we have recently extended our method to include substrates the height profile of which varies temporally in a prescribed manner.

We compare two cases: First, we investigate a droplet on substrates with planar-wave wettability pattern by varying the speed and wave length of the pattern. Second, we investigate a droplet on substrates with a planar-wave height profile. In both scenarios, for small wave velocities the droplet moves steadily forward. In contrast, above a wave velocity the droplet performs steady oscillations. These speed oscillations correlate with oscillations in the shape of the droplet which decay linearly as a function of pattern speed.

CPP 45: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods

Time: Thursday 9:30–12:00 Location: ZEU 255

CPP 45.1 Thu 9:30 ZEU 255

Structural effects of many-body van der Waals interactions: from small molecules to polymers — •Raul Ian Sosa, Mario Galante, and Alexandre Tkatchenko — Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg City, Luxembourg.

Van der Waals (vdW) dispersion interactions are among the key determinants of structure, stability, and dynamics in a wide range of systems such as supramolecules, complex interfaces and low-dimensional nanostructures. Most commonly used approaches for incorporating vdW interactions in extended systems rely on pairwise approximations, neglecting the quantum many-body nature of molecular interactions [Quantum Chem. 114, 1157 (2014), Science. 350, 6257 (2015)]. Recent simulations which incorporate Many-Body Dispersion (MBD) show that a many-body description of van der Waals can be essential for properly describing extended molecules and molecular solids [Physical Review Letters. 108, 23 (2012)]. These effects often manifest themselves as increased ranges of interaction and collective dynamics in a way that is highly dependent on the molecular structure [Nat Comm. 11, 1651 (2020)]. Here we will present a systematic analysis on the impact that many-body interactions have on the range of van der Waals forces in polymers, one dimensional nanostructures and small molecules, making a particular emphasis on the structural dependence of such interactions.

CPP 45.2 Thu 9:45 ZEU 255

Bulk magneto-mechanical response of magnetic filaments in applied magnetic fields — •Deniz Mostarac and Sofia Kantorovich — Univesity of Vienna,Vienna,Austria

Incorporating magnetic nanoparticles within permanently cross-linked structures, opens up the possibility for synthesis of complex, highly magneto-responsive systems. Magnetic filaments (MFs) are polymer-like chains of magnetic, nano-sized colloids, and are a promising platform for engineering novel, magnetically controlled filtering and flow control elements in micro-fluidic devices. The interplay between central attraction forces, and anisotropic, dipolar interactions is the key factor when tuning the macroscopic response of MFs. In this contribution, we show that taking in to account nonlinear contributions to the magnetisation of super-paramagnetic colloids is essential to capture the bulk, magneto-mechanical response of MFs consisting of magnetisable colloids. In the presence of central attraction forces, we report substantial differences in the equilibrium structure of filament clusters, and the mechanical and magnetic response of filament suspensions, to static and time dependant magnetic fields. While on the level of a single filament, magneto-mechanical properties are in general more dependant on the crosslinking approach than on the magnetic nature of colloids, in bulk, the long-range nature of dipolar interactions in quasi-infinite systems makes up for a tremendous difference, and underlines the necessity of a sophisticated model of magnetic colloids that can be magnetised by the presence of magnetic and dipole fields.

CPP 45.3 Thu 10:00 ZEU 255

Improving the Electrochemically Assisted Surfactant Assembly of Vertically Aligned Mesoporous Silica Films — •Gilles Möhl[1,2], Samuel Fitch[2], Li Shao[2], Jonathan Rawle[3], Ralph Gilles[1], Guy Denuault[2], Tauqir Nasir[2], Yisong Han[4], Richard Beanland[4], Ruomeng Huang[2], Yasir Noori[2], Philip Bartlett[2], and Andrew Hector[2] — [1]FRM II/TUM, München, Deutschland — [2]UOS, Southampton, United Kingdom — [3]Diamond Light Source, Harwell, United Kingdom — [4]Warwick University, Coventry, United Kingdom

Mesoporous silica films are typically produced by evaporation-induced self-assembly (EISA), but vertical alignment of the pores to the substrate remains difficult. Hexagonal arrays of vertically aligned mesopores can be made by electrochemically assisted surfactant assembly (EASA). The self-assembly of a cationic surfactant (cetyltrimethylammonium bromide), which relies on the production of hydroxide species close to the substrate, also leads to the formation of spheroidal surface aggregates, limiting the obtainable film thickness to a few hundreds of nm. In this work, we show the results obtained from operando Grazing incidence small angle X-ray scattering (GISAXS) experiments done during the EASA of silica, following the evolution of the structure formation in real time with sub-second time resolution. We include the findings from operando pH measurements using an electrochemical microsensor, revealing the temporal evolution of the hydroxide concentration close to the electrode. This enabled us to adapt the EASA protocol to reduce aggregate formation and increase film thickness.

CPP 45.4 Thu 10:15 ZEU 255

Pair-wise dependences of morphological descriptors provide fingerprint of pore structure in cellulose-based materials — •Karin Zojer[1], Matthias Neumann[2], Phillip Gräfensteiner[2], Eduardo Machado Charry[1], Andre Hilger[3], Ingo Manke[3], Ulrich Hirn[4], and Volker Schmidt[2] — [1]Institute of Solid State Physics,Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [2]Institute of Stochastics, Ulm University, Helmholtzstrasse 18, 89069 Ulm, Germany — [3]Institute of Applied Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [4]Institute of Bioproducts and Paper Technology, Graz University of Technology, Inffeldgasse 23, 8010 Graz, Austria

Predicting the macroscopic behavior of heterogeneous porous materials from their microscopic structure is formidably challenging, because local morphological microstructure descriptors markedly and erratically vary across a sample. We demonstrate how to quantify cross relationships between pore space-related descriptors and to use these relations to distinguish complex pore spaces at a glance, alike using fingerprints. The key idea is to map the actual microstructure on a multivariate probability distribution. The latter contains strongly compressed information to reproduce the spatial variations of selected properties and their pair-wise interdependencies. Using R-vine copulas, we will exemplarily construct such a distribution of the local morphological descriptors porosity, thickness, surface area per volume and pathway tortuosity for the measured microstructure of paper sheets.

CPP 45.5 Thu 10:30 ZEU 255

***Ab initio* cavity QED - modifying chemistry with strong light-matter interaction** — •Christian Schäfer[1,2], Enrico Ronca[3], Johannes Flick[4,5], Prineha Narang[5], and Angel Rubio[2,4] — [1]Department of Microtechnology and Nanoscience, MC2, Chalmers University of Technology, 412 96 Göteborg, Sweden — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [3]Istituto per i Processi Chimico Fisici del CNR (IPCF-CNR), Via G. Moruzzi, 1, 56124, Pisa, Italy — [4]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [5]John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts 02138, USA

The alchemical dream of altering a given material on demand into something desirable is at the very heart of chemistry. Optical-Cavity environments provide a novel handle to non-intrusively control materials and chemistry. The self-consistent interaction between complex electromagnetic environments and realistic materials gave birth to a new discipline, sometimes referred to as '*ab initio* QED', on the interface of condensed matter, chemistry and quantum optics.

I will provide a brief introduction into this newly emerged field and illustrate how chemical reactions can be controlled [1] with optical cavities.

[1] Schäfer, C., Flick, J., Ronca, E., Narang, P., and Rubio, A., arXiv:2104.12429 (2021).

CPP 45.6 Thu 10:45 ZEU 255

Structural Descriptors for Constructing High-Dimensional Neural Network Potentials — •Moritz R. Schäfer[1,2], Jonas A. Finkler[3], Stefan Goedecker[3], and Jörg Behler[1,2] — [1]Lehrstuhl für Theoretische Chemie II, Ruhr-Universität Bochum, 44780Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research AllianceRuhr, 44780 Bochum, Germany — [3]Basel University, Department of Physics, Klingelbergstrasse 82, 4056 Basel, Switzerland

High-dimensional neural network potentials (HDNNPs) are a well established method to efficiently compute close-to ab initio-quality energies and forces for performing large-scale molecular dynamics simulations of complex systems. In this method, the total energy is constructed as a sum of environment-dependent atomic energy contributions. Also electrostatic interactions based on flexible atomic charges can be included. Both components crucially depend on the quality of the structural descriptors employed to characterize the local atomic environments. Here we investigate the combination of atom-centered symmetry functions with the recently proposed overlap matrix descriptor. Moreover, the advantages and disadvantages of both descriptors are discussed and illustrated for benchmark systems.

CPP 45.7 Thu 11:00 ZEU 255

Solving inverse transport problems across irregular interfaces of sorptive porous media via physics-informed neural networks — •Alexandra Serebrennikova and Karin Zojer — Institute of Solid State Physics, TU Graz, Petersgasse 16, 8010, Graz, Austria

We show how state of the art extended physics-informed neural networks serve us to solve inverse transport problems with jump conditions across irregular interfaces. This approach reveals the material constants which govern reactive diffusion of organic volatiles migrating across an interface between porous sorptive packaging and food media if we provide experimental data and a transport model.

In such scenarios, associated differential equations (PDE) imply jumps not only in the solution, but also in the solution gradient across interfaces. The idea is to use multiple NN to construct the solution; each NN approximates the solution function of the PDE associated to a domain within the defined interfaces. The networks are coupled across interfaces such that the boundary conditions are satisfied.

As NNs are required to fit underlying physics by minimizing PDE residuals, they are inherently suited to solve inverse problems for the parameters involved in the equations. As further benefit, the discretized experimental data can be represented with a continuous function which offers a meshfree and compact surrogate model for the solution function.

15 min. break

CPP 45.8 Thu 11:30 ZEU 255

Aging-driven compositional changes in Li-ion batteries — •Dominik Petz[1,2], Peter Müller-Buschbaum[1,2], and Anatoliy Senyshyn[1] — [1]MLZ, TUM, Garching — [2]TUM School of Natural Sciences, Chair of Functional Materials, Garching

Electrochemical cycling of lithium-ion batteries is supplemented by the active transport of lithium ions and electrons, which are exchanged between the cathode and anode material. Besides material properties, such exchange is facilitated by the parameters of electrochemical cell like electrode dimensions and geometry, current density, temperature, etc. Such parameters are neither uniformly distributed nor static in general and, therefore, serve as a factor stabilizing heterogeneous states in Li-ion batteries typically reflected in the lithium concentration profiles in the electrodes. Thus, cell aging directly affects the distribution of the lithium-ions in the graphite anode of 18650-type lithium-ion batteries. Lithium heterogeneities (often reflected in loss of lithium inventory) are directly related to the electrolyte filling level. In order to quantify and correlate them simultaneously, a set of cells at different state-of-health was studied non-destructively using spatially resolved neutron powder diffraction. Experimental results unambiguously revealed changes of the lithium and electrolyte distribution versus cell state-of-health in a series of commercial 18650-type lithium-ion battery.

CPP 45.9 Thu 11:45 ZEU 255

Dedoping of PEDOT:PSS using amines to shift the threshold voltage in OECTs — •Laura Teuerle, Rakesh Nair, Hans Kleemann, and Karl Leo — IAPP Dresden

With an increasing importance of organic semiconductors, due to their flexibility, transparency and possible biocompatibility, more applications and device classes emerge.

One of them - the organic electochemical transistor (OECT) can be utilized in neuromorphic computing and printed digital logic. The most commonly used -PEDOT:PSS is a p-type semiconductor, which leads to normally-on type transistors. However, normally-off type devices are needed for a successful application in logic circuits.

We show that a chemical dedoping method involving amines leads to a shift in threshold voltage to zero and even negative in the corresponding devices.

Different processing methods for the dedoping process and device building are studied, which involve photolithography, inkjet printing and spraycoating.

Furthermore, IV measurements for device characterization were taken.

The results show that the studied chemical dedoping of -PEDOT:PSS can be a viable method to create normally-off type transistors for an application in logic circuits.

CPP 46: Active Matter IV (joint session DY/BP/CPP)

Time: Thursday 9:30–13:00 Location: ZEU 160

Invited Talk CPP 46.1 Thu 9:30 ZEU 160

Acoustically propelled nano- and microparticles: From fundamentals to applications — •Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Among the existing types of artificial active colloidal particles, acoustically propelled nano- and microparticles have a particularly high potential for future applications in fields like medicine and materials science. However, despite intensive research on this type of motile particles in recent years, the understanding of their properties is still very limited. A reason for the limited understanding is that the previous research has mostly been experimental and that it is difficult to study the dependence of certain system parameters on the propulsion of the particles in experiments since the parameters can often not be varied independently of the other parameters and in ranges of reasonable size. In this talk, I will give an overview about our theoretical investigation of the properties of acoustically propelled nano- and microparticles and the challenges that remain for future research.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – 283183152 (WI 4170/3).

CPP 46.2 Thu 10:00 ZEU 160

Force on probe in a confined active fluid — Shuvojit Paul[1], •Ashreya Jayaram[2], N Narinder[1], Thomas Speck[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, 78464 Konstanz, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany

When immersed in a dispersion of smaller ”depletants”, a colloidal particle experiences depletion forces in the presence of another colloidal particle or under confinement. While the nature of these forces is well-established for passive systems, much less is known about the consequence of making the depletants self-propelled or ”active”. In this work, we consider a large, optically trapped probe under circular confinement surrounded by smaller active Janus particles. We find that the force experienced by the probe varies non-monotonically as the distance between the colloid and the confinement is increased. To rationalize this observation, we relate the measured force to the active stress and, subsequently, to the microstructure of the surrounding active fluid. Going beyond synthetic active matter, our work could shed light on the organization of intracellular entities in biological systems.

CPP 46.3 Thu 10:15 ZEU 160

Symmetry-breaking refractive index profiles as a propulsion mechanism for active Brownian particles — •Julian Jeggle[1], Matthias Rüschenbaum[2], Cornelia Denz[2], and Raphael Wittkowski[1] — [1]Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Institut für Angewandte Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Active Brownian particles (ABPs) have been realized with various propulsion mechanisms such as self-diffusiophoresis, self-electrophoresis or acoustic scattering. Typically, these mechanisms induce flow fields around the particles that represent a deviation from the “pure” ABP model. Here, we present a novel implementation of ABPs in the form of transparent microswimmers with a symmetry-breaking refractive index gradient. Utilizing the momentum transfer associated with light refraction as the driving force induces no flow fields beyond Stokes flow. Unlike optothermally driven particles, this archetype of ABPs also allows for sensitivity to the phase and polarization of the driving light field thus improving the spatio-temporal control of light-based propulsion mechanisms. Using non-light-absorbing particles enables bulk volume systems and allows the introduction of feedback loops, therefore making this approach a promising foundation for adaptive matter systems.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – Project-ID 433682494 - SFB 1459

CPP 46.4 Thu 10:30 ZEU 160

The interaction-expansion method: a systematic derivation strategy for active field theories* — •Michael te Vrugt[1,2], Jens Bickmann[1,2], Stephan Bröker[1,2], Tobias Frohoff-Hülsmann[1], Eyal Heifetz[3], Michael E. Cates[4], Uwe Thiele[1,5,6], and Raphael Wittkowski[1,2,5] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]SoN, Westfälische Wilhelms-Universität Münster — [3]Porter School of the Environment and Earth Sciences, Tel Aviv University, 69978 Tel Aviv, Israel — [4]DAMTP, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom — [5]CeNoS, Westfälische Wilhelms-Universität Münster — [6]CMTC, Westfälische Wilhelms-Universität Münster

Field-theoretical models have made enormous contributions to our understanding of the collective dynamics of active matter. In this contribution, we introduce the interaction-expansion method (IEM) [1], which allows for a systematic derivation of active field theories from the microscopic dynamics of individual particles. We then discuss some recent applications of the IEM to particles with orientation-dependent propulsion speed [2] and particles with inertia [3].

[1] M. te Vrugt et al., in preparation (2022)

[2] S. Bröker et al., arXiv:2210.13357 (2022)

[3] M. te Vrugt et al., Nature Communications (provisionally accepted), arXiv:2204.03018 (2022)

**Funded by the Deutsche Forschungsgemeinschaft (DFG)– 283183152*

CPP 46.5 Thu 10:45 ZEU 160

Entropy production in active turbulence — •Byjesh Nalini Radhakrishnan, Thomas Schmidt, and Etienne Fodor — Department of physics and material science, University of Luxembourg

Active particles like bacteria and sperm cells sustain a continuous intake and dissipation of energy. Consequently, they are intrinsically out of equilibrium which leads to a non-vanishing entropy production rate (EPR) even in steady states. Quantifying how the EPR varies in different collective phases is crucial in developing a thermodynamic framework for active matter. In this work, we look at the EPR in active turbulence. We use Active Model H, a continuum model for active particles in a momentum-conserving fluid, to study turbulence in contractile scalar active systems. We measure the local EPR in numerical simulations, which unveils the role of the noise and activity parameters on the EPR in active turbulent systems.

15 min. break

CPP 46.6 Thu 11:15 ZEU 160

Phase transitions in multicomponent active matter: a quantitative kinetic theory — •Jakob Mihatsch[1], Thomas Ihle[1], Rüdiger Kürsten[2], and Horst-Holger Boltz[1] — [1]Institute for Physics, University of Greifswald, Greifswald, Germany — [2]Departament de Física de la Matèria Condensada, University of Barcelona, Barcelona, Spain

We consider a multicomponent model of self-propelled particles with Kuramoto-type alignment interactions. Starting from the N-particle Fokker-Planck equation we observe that the usual factorization Ansatz of the probability density, often called Molecular Chaos approximation, predicts a relaxation behavior which qualitatively disagrees with agent-based simulations. Therefore, we develop a kinetic theory which takes the time-evolution of the two-particle correlation function explicitly into account, i.e. goes beyond the mean-field approximation. We show that this theory predicts the relaxation behavior of the system as well as the order-disorder transition with high precision in certain parameter ranges. In particular, the dependence of the transition threshold on the particle speed is predicted correctly.

CPP 46.7 Thu 11:30 ZEU 160

Emergent collective behaviour due to virtual interactions between robotic swimmers — •Samudrajit Thapa[1,2], Bat-El Pinchasik[1,3], and Yair Shokef[1,2,3] — [1]School of Mechanical Engineering, Tel Aviv University, Tel Aviv 69978, Israel — [2]Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv 69978, Israel — [3]Center for the Physics and Chemistry of Living Systems, Tel Aviv University, 69978, Tel Aviv, Israel

Many organisms in nature use local interactions to realize global collective behaviour. Here we study how simple two body distance-based interactions between active Brownian particles results in collective motion. The interactions are not physical but virtual, wherein each particle senses the presence of other particles nearby and changes its behaviour accordingly. We study the radial distribution function to quantify the emergent interactions for both social and anti-social behaviour. Using Langevin dynamics simulations, we discover that under certain conditions positive correlations of the motion can emerge even in the case of anti-social behaviour. Our results might be potentially useful for designing robotic swimmers that can swim collectively just based on sensing the distance to their neighbours.

CPP 46.8 Thu 11:45 ZEU 160

Kinetic Event-Chain Algorithm for Active Matter

— •Nico Schaffrath, Thevashangar Sathiyanesan, Tobias Kampmann, and Jan Kierfeld — Physics Department, TU Dortmund University, 44221 Dortmund, Germany

We present a cluster kinetic Monte-Carlo algorithm for active matter systems of self-propelled hard particles. The kinetic event-chain algorithm is based on the event-chain Monte-Carlo method and is applied to active hard disks in two dimensions. The algorithm assigns Monte-Carlo moves of active disks a mean time based on the mean and variance of the move length in force direction. This time is used to perform diffusional rotation of their propulsion force. We show that the algorithm reproduces the motility induced phase separated region in the phase diagram of hard disks correctly and efficiently.

CPP 46.9 Thu 12:00 ZEU 160

Emergent pattern formation in communicating active matter

— •Robert Grossmann[1], Zahra Mokhtari[2], Robert I.A. Patterson[3], and Felix Höfling[2,4] — [1]Institut für Physik und Astronomie, Universität Potsdam — [2]Institut für Mathematik, Freie Universität Berlin — [3]WIAS Berlin — [4]Zuse Institut Berlin

Inspired by trail formation as observed in colonies of driver ants, for example, we study ensembles of agent particles that communicate via deposition and sensing of pheromones. These chemical traces are produced by the agents themselves and encode their current position and walking direction. Other agents passing by will then tend to align with the orientation inscribed in the pheromone traces. In the limit of short pheromone lifetime, the dynamics of this system reduces to the seminal Vicsek model and, thus, yields the formation of transversally moving bands. In the opposite limit, the effective agent-agent interaction represents a form of delayed feedback and yields the spontaneous formation of macroscopic, persistent trails, which are followed and reinforced by the agents [New J. Phys. **24** 013012 (2022)]. In this talk, we present large-scale simulations of the agent model and establish the phase diagram as function of the lifetime of pheromones. We rationalize our findings by analyzing mean-field equations that are systematically derived from the stochastic particle model. Combining numerical solutions of these order parameter equations and a linear stability analysis, we show how transversal bands, common in the Vicsek model, are destabilized, giving rise to the formation of "longitudinal" trails, pointing in the mean direction of motion.

CPP 46.10 Thu 12:15 ZEU 160

Binary Mixture of Deforming Particles

— •Yiwei Zhang, Alessandro Manacorda, and Etienne Fodor — DPhyMS, University of Luxembourg, Luxembourg, Luxembourg

Phase separation occurs in miscible liquids where components have distinct properties. In reactors, components undergo stochastic change in their properties which affect the liquid composition. While phase separation and reaction-diffusion have already been studied extensively as separate ingredients, how they combine in non-ideal reactors remains poorly understood. To bridge this gap, we consider repulsive particles with fluctuating size subject to one-body landscape and nonequilibrium synchronisation. The landscape features minima which, regarding size as reaction coordinate, distinguish three states: Particles with finite size, either A- or B-type, and point particles. In this context, synchronisation penalizes A particles in B-rich phases, and vice versa, so that the system eventually accommodates a uniform state. We report the phase diagram depending on the stability of each state and the corresponding particle sizes. Combining hydrodynamic and phenomenological arguments, we recapitulate how metastability regulates the interplay between synchronisation and repulsion. Our results reveal the role of nonequilibrium kinetic factors at play in non-ideal reaction-diffusion systems.

CPP 46.11 Thu 12:30 ZEU 160

Self-organization of model catalytic cycles

— •Vincent Ouazan-Reboul[1], Jaime Agudo-Canalejo[1], and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, D-37077, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, OX1 3PU, Oxford, UK

We study analytically and numerically a model metabolic cycle composed of an arbitrary number of species of catalytically active particles. Each species converts a substrate into a product, the latter being used as the substrate by the next species in the cycle. Through a combination of catalytic activity and chemotactic mobility, the catalytic particles develop effective interactions with particles belonging to neighbouring species in the cycle. These interactions, being fully out-of-equilibrium, show some unusual features, in particular being non-reciprocal. We find that such model metabolic cycles are able to self-organize through a macroscopic instability, with a strong dependence on the characteristics of the cycle. For instance, cycles containing an even number of species are able to minimize repulsion between their component particles by aggregating all even-numbered species in one cluster, and all odd-numbered species in another. Such a grouping is not possible if the cycle contains an odd number of species, which can lead to oscillatory steady states in the case of chasing interactions.

CPP 46.12 Thu 12:45 ZEU 160

Reentrant condensation transition in a model of driven scalar active matter with diffusivity edge

— Berx Jonas[2], •Bose Aritra[1], Mahault Benoit[1], and Golestanian Ramin[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany — [2]Institute for Theoretical Physics, KU Leuven, B-3001 Leuven, Belgium — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

A class of scalar active matter for which the effective diffusivity vanishes beyond a certain density threshold, hereby referred to as diffusivity edge, triggers the formation of a condensate when confined in a harmonic potential. The condensation transition exhibits remarkable similarities with a Bose-Einstein Condensation (BEC). Here we study the effect of a diffusivity edge in a system of scalar active matter confined by a periodic potential and driven by an external force.

We find that this system shows qualitatively distinct stationary regimes depending on the amplitude of the driving force with respect to the potential barrier. For small driving, the diffusivity edge induces a condensation analogous to the BEC-like transition reported for the nondriven case, which is characterised by a density-independent steady state current. Conversely, large external forces lead to a qualitatively different phase diagram where condensation is not possible below a density threshold and the associated transition at moderate densities above the threshold the transition is reentrant due to the existence of a subsequent evaporation transition at low effective temperatures.

CPP 47: 2D Materials VI (joint session HL/CPP)

Time: Thursday 9:30–12:00 Location: POT 81

CPP 47.1 Thu 9:30 POT 81

Negative differential resistance with ultra-high peak-to-valley current ratio in tunnel diodes based on two-dimensional cold metals — •Ersoy Sasioglu and Ingrid Mertig — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, 06120 Halle (Saale)

The negative differential resistance (NDR) effect is of great interest for future memory and logic circuit applications. We propose a novel semiconductor-free NDR tunnel diode concept with ultra-high peak-to-valley current ratio (PVCR) [1]. Our proposed NDR diode consists of two cold metal electrodes separated by a thin insulating tunnel barrier. The NDR effect stems from the unique electronic band structure of the cold metal electrodes, i.e., the width of the isolated metallic bands around the Fermi level as well as the energy gaps separating higher- and lower-lying bands determine the current-voltage characteristics and PVCR value of the tunnel diode. By proper choice of the cold metal electrodes either Λ-type or N-type NDR effect can be obtained. We employ the nonequilibrium Green's function method combined with density functional theory to demonstrate the NDR characteristics of the proposed diode based on two-dimensional NbS$_2$/h-BN/NbS$_2$ vertical and AlI$_2$/MgI$_2$/AlI$_2$ planar heterojunctions. For the lateral tunnel diode, we obtain a Λ-type NDR effect with an ultra-high PVCR value of 10^{16} at room temperature, while the vertical tunnel diode exhibits a conventional N-type NDR effect with a smaller PVCR value of about 10^4. The proposed concept provides a semiconductor-free solution for NDR devices to achieve desired I-V characteristics.

[1] Ersoy Şaşıoğlu and Ingrid Mertig, arXiv:2207.02593 (2022).

CPP 47.2 Thu 9:45 POT 81

Electrical contact engineering on 2D material through ion implantation and flash lamp annealing — •kaiman lin[1,2], yi li[2], manfred helm[2], shengqiang zhou[2], yaping dan[1], and slawomir prucnal[2] — [1]University of Michigan-Shanghai Jiao Tong University Joint Institute, Shanghai Jiao Tong University, 20024 Shanghai, P. R. China — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

In recent years, 2D material-based nanodevices have been extensively studied and exhibit highly competitive performance compared with conventional bulk semiconductors. Before they can be fully integrated with existing Si-based technology or offer new platform for novel nanoelectronics, some challenges must be solved. One of the key challenges in 2D devices is the large Schottky barrier at the 2D/metal interface, which limits the charge carrier injection from metal to 2D channel. In this paper, we propose a novel method, which exploits the top metal electrode as the capping layer during the ion implantation process, followed by ms-range flash lamp annealing to repair the defects caused by ion implantation and to activate dopants. Our approach allows to realize effective doping at the interface between multilayer 2D materials and metal electrodes and simultaneously minimize the defect concentration created during the ion implantation process. As a result, the ohmic contact between 2D material and metal electrodes will be realized.

CPP 47.3 Thu 10:00 POT 81

Impact of free carriers on exciton and trion diffusion in monolayer WSe2 — •Marzia Cuccu[1], Koloman Wagner[1], Zakhar A. Iakovlev[2], Jonas D. Ziegler[1], Takashi Taniguchi[3], Kenji Watanabe[3], Mikhail M. Glazov[2], and Alexey Chernikov[1] — [1]TU Dresden, Dresden, Germany — [2]St. Petersburg, Russia — [3]National Institute for Materials Science, Tsukuba, Japan

In monolayer transition metal dichalcogenides excitons are tightly bound, mobile at room and cryogenic temperatures, and interact strongly with free charge carriers. However, the role of the exciton-electron interaction in the context of exciton propagation remains unclear. Here, we address this question by demonstrating diffusion of excitons in hBN-encapsulated WSe2 in the presence of a continuously tunable Fermi sea. Using ultrafast microscopy, we reveal a non-monotonic dependence of the exciton diffusion coefficient on the charge carrier density in both electron- and hole-doped regimes. We identify distinct regimes of elastic scattering and quasiparticle formation determining exciton diffusion and highlight the importance of treating exciton-electron scattering in the presence of additional energy and momentum dissipation via phonons. We further show that trions remain mobile even at low temperatures down to 5 K, with an effective trion mobility up to 3000 cm2/(Vs).

CPP 47.4 Thu 10:15 POT 81

Electrical Characterization of Thin ZrSe$_3$ Films — •Lars Thole[1], Christopher Belke[1], Sonja Locmelis[2], Peter Behrens[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany

Two dimensional materials have been of great interest in the past years, because of their huge potential for new applications [1]. While graphene has been extensively researched, a lot of other materials have emerged. One of the most notable groups are the transition metal chalcogenides because of their variety of different compounds. Among these the lesser known transition metal trichalcogenides show unique properties [2].

Here, we have researched the transition metal trichalcogenide ZrSe$_3$ [3]. Its bulk material was produced by a chemical vapor transport method and was then exfoliated to obtain thin films. Electrical measurements show a band gap of 0.6 eV which increases for thinner samples. The material is shown to be an n-type semiconductor by transistor measurements and a mean free path of about 103 nm was determined by looking at different samples with varying thicknesses.

[1] A. K. Geim, I. V. Grigorieva, Nature, 499, 419-425 (2013).
[2] J. O. Island et al., 2D Materials, 4, 0220033 (2017).
[3] L. Thole et al., ACS Omega, 7, 39913 (2022).

CPP 47.5 Thu 10:30 POT 81

Electrically active deep defects in 2D vdW semiconductors — •Michele Bissolo[1], Rongxin Li[1], Masako Ogura[2], Svitlana Polesya[2], Hubert Ebert[2], Eugenio Zallo[1], Gregor Koblmüller[1], and Jonathan J. Finley[1] — [1]Walter Schottky Institute and TUM School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany — [2]Department of Chemistry/Phys. Chemistry, LMU Munich, Butenandtstrasse 11, 81377 Munich, Germany

Mid-gap defect states in semiconductors can both potentially degrade the performance of (opto)electronic devices and simultaneously act as a platform for technologies such as (photo)catalysis and quantum computing. Characterizing the electrically active mid-gap defects in the emerging class of 2D van-der-Waals materials is thus a necessary step in the development of future 2D-based devices. Here, we employ Deep Level Transient Spectroscopy (DLTS) techniques to directly probe deep defects in transition metal dichalcogenides (TMDCs) and group-III monochalcogenides (III-MCs), which have recently gained traction in "more-than-Moore", low-power and renewable energy device applications. Unlike transmission electron or scanning tunneling microscopies, DLTS is both a non-destructive and bulk sensitive technique that provides multiple information on the electronically active defect states, such as concentration, energy and capture cross section. DLTS spectra are collected from few-layer MoS$_2$, MoSe$_2$ and GaSe Schottky diodes in the 10-300 K temperature range with 10 mK stability, and the properties and role of the observed defects are discussed.

15 min. break

CPP 47.6 Thu 11:00 POT 81

Ionic based gate control of insulator-to-metal phase transitions on ZrS$_2$ — •Jose Guimaraes[1,2], Dorsa Fartab[1], Marcus Schmidt[1], and Haijing Zhang[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]School of Physics and Astronomy, University of St Andrews, St Andrews KY16 9SS, UK

The possibility of tuning the properties of solids, such as their carrier density, allows for the amplification of their potential: In the context of 2D materials, ionic liquid gating provides a highly efficient doping alternative to traditional chemical doping.

Transitional metal dichalcogenides (TMDCs) have emerged as a potential 2D replacement for silicon in many technological applications, however their carrier mobility needs to be vastly increased. Ionic liquid gating enables carrier concentrations of the order of 10^{14} carriers per cm^2 in certain TMDCs, moreover, it allows for the emergence of unique physical phenomena, such as ambipolar behaviour. To realize transistor applications, materials that can be easily switched between p-type and n-type by applying an electric field are essential to minimize circuit size.

Here, an overview of the ionic liquid gating technique is given, including device fabrication and characterization methods, focusing on the TMDCs: ZrS_2 and $ZrSe_2$. Being $ZrSe_2$ an oxygen sensitive material, a method of estimating its thickness by its optical image is discussed. Furthermore, experimental efforts reporting ambipolar behaviour in ZrS_2 for the first time are presented.

CPP 47.7 Thu 11:15 POT 81

Lattice reconstruction in twisted transition metal dichalcogenide heterobilayers — •Wei Li, Thomas Brumme, and Thomas Heine — TU Dresden, Dresden, Germany

Twisted heterostructures of 2D crystals have resulted in a series of high-impact contributions to condensed matter physics, most prominently flat bands and superconductivity in twisted bilayer graphene. But also two-dimensional crystals beyond graphene, such as transition metal dichalcogenides, show strong proximity effects that are affected by twisting. Here, we systematically investigate the structural impact of twist angles on transition metal dichalcogenide van der Waals heterobilayers consisting of MoS_2, WS_2, $MoSe_2$ and WSe_2 monolayers. We find that the significant lattice reconstruction involving in- and out-of-plane displacements strongly depends on the twist angle: from a continuous variation of local stacking alignment at large twist angles to a soliton-domain structure at small twist angles. Especially, starting from either 2H or 3R stacking, two different critical twist angles exist, above which the two constituting layers show dramatically asymmetrical corrugation, in contrast to the symmetry-preserving out-of-plane deformation in twisted homobilayers. We reveal that the development of either the corrugation or the soliton-domain results from the competition between strain energy cost and van der Waals energy gain. Our calculations show that van der Waals heterobilayers develop, besides the well-investigated moiré structures, also systems with large areas of special local stackings arranged in a superlattice, suggesting intriguing electronic properties of these systems.

CPP 47.8 Thu 11:30 POT 81

Pump Probe Signatures of Interlayer Excitons in TMDC Heterostructures — •Henry Mittenzwey[1], Manuel Katzer[1], Benjamin Kaiser[2], Veronica Policht[3], Oleg Dogadov[3], Stefano Dal Conte[3], Giulio Cerullo[3], Andreas Knorr[1], and Malte Selig[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Zuse Institute Berlin, Takustraße 7, 14195 Berlin, Germany — [3]Dipartimento di Fisica, Politecnico di Milano, I-20133 Milano, Italy

TMDC heterobilayers are promising candidates for novel optoelectronic applications, since they exhibit long-lived excitonic states with spatially separated electrons and holes located in different layers. The relaxation dynamics of these interlayer excitons and their interplay with intralayer excitons are still under investigation.

Here, we present a microscopic description for the phonon and tunneling induced formation and relaxation of intra- and interlayer excitons in a $MoSe_2/WSe_2$ stack. Based on the microscopic dynamics we calculate the pump probe signal for intra- and interlayer transition and their population dynamics including hot exciton bottleneck effects and unbound interlayer occupations.

CPP 47.9 Thu 11:45 POT 81

Microscopic picture of interlayer exciton-phonon coupling — Muralidhar Nalabothula, Ludger Wirtz, and •Sven Reichardt — University of Luxembourg, Luxembourg

Excitons play a key role for opto-electronic applications of 2D heterostructures. They also can strongly couple to phonons as evidenced by their imprint on resonant Raman scattering intensities [1,2]. In 2D heterostructures, this sort of strong coupling and its signature Raman scattering offers an ideal setting to learn about exciton-phonon coupling both within and across material layers. Here we focus on the example of monolayer WSe2 and hBN. Its Raman spectrum features the norminally silent out-of-plane optical phonon mode of hBN that becomes active due to symmetry breaking and - most curiously - very strongly enhanced due to resonant exciton-phonon scattering [1]. While the resonant scattering pathways have been identified as involving excitons in WSe2 that couple to the phonons in hBN [1], a microscopic understanding of this interlayer exciton-phonon coupling is still missing. We provide such understanding using the state-of-the-art method for the computation for resonant Raman scattering intensities [2,3], which allows a detailed atomistic and quantum mechanical dissection of the Raman scattering process. Supplemented by a classical picture, our work sheds light on the microscopic mechanism behind exciton-phonon coupling in 2D heterostructures.

[1] C. Jin, et al. Nat. Phys., 13, 127-131, (2017).

[2] S. Reichardt and L. Wirtz. Sci. Adv. 6, eabb5915, (2020).

[3] S. Reichardt and L. Wirtz. Phys. Rev. B 99, 174312, (2019).

CPP 48: Data Driven Materials Science: Big Data and Work Flows – Microstructure-Property-Relationships (joint session MM/CPP)

Time: Thursday 10:15–13:15 Location: SCH A 251

CPP 48.1 Thu 10:15 SCH A 251

Orisodata: A methodology for grain segementation in atomistic simulations using orientation based iterative self-organizing data analysis — •Arun Prakash — Micro-Mechanics and Multiscale Materials Modeling (M5), TU Bergakademie Freiberg

Atomistic simulations of the molecular statics/dynamics kind have established themselves as a cornerstone in the field of computational materials science. Large scale simulations with tens to hundreds of millions of atoms are regularly used to study the behavior of nano-(poly)crystalline materials. Identifying grains a posteriori in such simulations is a challenging task, particularly for simulations at high temperatures or at large strains. In this work, we propose a methodology for grain segmentation of atomistic configurations using unsupervised machine learning [1]. The proposed algorithm, called OrISODATA, is based on the iterative self-organizing data analysis technique and is modified to work in the orientation space. The algorithm is demonstrated on a 122 grain nanocrystalline thin film sample in both undeformed and deformed states. The Orisodata algorithm is also compared with two other grain segmentation algorithms available in open-source visualization tool Ovito. The results show that the Orisodata algorithm is able to correctly identify deformation twins as well as regions separated by low angle grain boundaries. The intiutive model parameters relate to similar thresholds in experiments, which helps obtain optimal values and facilitates easy interpretation of results.

References: [1]: M. Vimal, S. Sandfeld and A. Prakash [2022]: Materialia, 21, 101314

CPP 48.2 Thu 10:30 SCH A 251

Comparison of atomic environment descriptors with domain knowledge of the interatomic bond — •Mariano Forti, Ralf Drautz, and Thomas Hammerschmidt — ICAMS, Ruhr Universität Bochum, Universität Straße 150, 44801 Bochum

The study of the relative stability of multicomponent materials and the search for new materials for high performance applications requires extensive samplings of the composition space. This is a demanding task due to the computational effort that is required for the electronic structure calculations. In this work we propose a machine learning approach with descriptors of the local atomic environment using different chemistry heuristics based on smooth overlap of atomic positions, recursive solutions of tight-binding Hamiltonians and atomic cluster expansions. We demonstrate that these descriptors, which retain different levels of domain knowledge of structural and electronic properties of the chemical compounds, can be used to predict formation energies with high accuracy even with simple regression algorithms. We apply the methodology to complex crystal structures in binary and ternary intermetallic systems.

CPP 48.3 Thu 10:45 SCH A 251

A Machine-Learning Framework to Identify Equivalent Atoms at Real Crystalline Surfaces — •King Chun Lai, Sebastian Matera, Christoph Scheurer, and Karsten Reuter — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Functional surfaces and interfaces even of crystalline materials are characterized by breaks of symmetry and long-range order. Yet, even though such a crystalline surface may for instance exhibit numerous vacancies, adatoms, steps, kinks or islands, there are generally still many equivalent atoms, where equivalence refers to an identical or near-identical local environment. There are many equivalent terrace atoms, adatoms, step or kink atoms. In atomic-scale modeling and simulation, identifying these groups of equivalent atoms is a routine task, not least because one would e.g. restrict demanding first-principles calculations like the determination of an adsorption configuration and concomitant adsorption energy to only one site of each equivalence group. Aiming to automatize this routine task, we here present a machine-learning framework to identify all groups of equivalent atoms for any surface or nanoparticle geometry. The initial classification rests on the representation of the local atomic environment through a high-dimensional smooth overlap of atomic positions (SOAP) vector. We then achieve a fuzzy classification by mean-shift clustering within a low-dimensional embedded representation of the SOAP points as obtained by multidimensional scaling (MDS). The performance of this classification framework will be demonstrated with examples of Pd surfaces.

CPP 48.4 Thu 11:00 SCH A 251

Identifying ordered domains in atom probe tomography using machine learning — •Alaukik Saxena, Navyanth Kusampudi, Shyam Katnagallu, Baptiste Gault, Dierk Raabe, and Christoph Freysoldt — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf 40237, Germany

Atom probe tomography (APT) is a unique technique that provides 3D elemental distribution with near-atomic resolution for a given material. The spatial resolution of APT is ~1-3 Å in depth and ~3-5 Å in the lateral direction, respectively. Due to the limited spatial resolution, most of the APT data analysis focuses on composition to extract various microstructural features. Here, we aim at identifying additional on-lattice short-range order within an Al-Mg-Li alloy even though the underlying FCC lattice itself is not resolved. We propose a machine learning (ML) methodology to distinguish disordered solid solutions from ordered L12 domains. To encapsulate the local chemistry and noisy structure in APT independent of orientation, we use Smooth Overlap of Atomic Positions (SOAP). To find suitable hyperparameters of the high-dimensional SOAP features, we visualize the data distribution within the latent space of an auto-encoder neural network trained on experimental data with a preliminary classification. After the optimization, synthetic data corresponding to FCC and L12 structures is created with APT level spatial noise and then used for training from scratch a dense neural network for order/disorder classification. The trained model is then able to distinguish between ordered and disordered structures in experimental data.

CPP 48.5 Thu 11:15 SCH A 251

Atomic cluster expansion: training a transferable water interatomic potential from the local atomic environments of ice — •Eslam Ibrahim, Yury Lysogorskiy, Matous Mrovec, and Ralf Drautz — ICAMS, Ruhr Universität Bochum, 44780 Bochum, Germany

We show the predictive power of the atomic cluster expansion (ACE) for modeling challenging systems such as water. We trained ACE on data from ab-initio molecular dynamics simulations (AIMD) of water at 300 K. ACE displays excellent agreement to the first-principles reference data in predicting radial distribution functions and covalent and hydrogen bonding characteristics. However, our investigation confirms that describing properties that require sampling a larger fraction of phase space, for example, self-diffusion or the free energies, requires longer AIMD simulation times at different pressures/densities and temperatures. We then show that ice structures provide a more efficient means of sampling the phase space of water: training ACE to diverse ice phases only describes liquid water in quantitative and qualitative agreement with first principles reference data. This reveals a powerful and efficient strategy for building transferable water interatomic potentials without running expensive AIMD.

15 min. break

CPP 48.6 Thu 11:45 SCH A 251

Enhancing molecular dynamics simulations of water in comparison to neutron scattering data with algorithms — •Veronika Reich[1], Luis Carlos Pardo[2], Martin Müller[3], and Sebastian Busch[1] — [1]GEMS at Maier-Leibnitz Zentrum, Helmholtz-Zentrum hereon, 85748 Garching, Germany — [2]Departament de Física Escola d'Enginyeria de Barcelona Est Universitat Politècnica de Catalunya, 08019 Barcelona, Spain — [3]Helmholtz-Zentrum hereon, 21502 Geesthacht, Germany

The structure and dynamics of materials can be studied on the atomic level with neutron and X-ray scattering experiments as well as molecular dynamics (MD) simulations. We connect experimental data with MD simulations to further enhance the simulations and obtain force-fields that are able to reproduce the measured structure and dynamics.

On the example of water, we established a workflow of running MD simulations in the program LAMMPS, calculating X-ray and neutron scattering data with the program Sassena, and comparing the diffractograms and incoherent intermediate scattering functions to already published experimental data.

The agreement between computed scattering curves and experimental data was optimized with algorithms to obtain a set of parameters that can simultaneously reproduce the real nanoscopic structure and dynamics of water probed by the neutron and X-ray scattering experiments.

This scheme is highly adaptable to different MD simulations of various models.

CPP 48.7 Thu 12:00 SCH A 251

Stress and Heat Flux via Automatic Differentiation — •Marcel F. Langer[1,2,3], Florian Knoop[3,4], J. Thorben Frank[1,2], Christian Carbogno[3], Matthias Scheffler[3], and Matthias Rupp[3,5] — [1]BIFOLD – Berlin Institute for the Foundations of Learning and Data, Berlin, Germany — [2]Machine Learning Group, Technische Universität Berlin, Germany — [3]The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society and Humboldt University, Berlin, Germany — [4]Theoretical Physics Division, Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden — [5]Materials Research and Technology Department, Luxembourg Institute of Science and Technology (LIST), Luxembourg

Computationally efficient approximations of the Born-Oppenheimer potential energy surface can be obtained by parametrising an analytical force field based on a set of reference calculations. Inspired by recent developments in machine learning, such potentials can include equivariant semi-local interactions through message-passing mechanisms and rely on automatic differentiation (AD), overcoming the need for manual derivative implementations or finite-difference schemes. We provide a unified framework for using AD in such state-of-the-art potentials, and discuss how AD can be used to efficiently and simply compute the stress tensor and the heat flux. We validate the framework by predicting thermal conductivity for selected semiconductors and insulators with an equivariant machine learning potential [1].

[1]: J.T. Frank, O.T. Unke, K.-R. Müller, arXiv 2205.14276 (2022).

CPP 48.8 Thu 12:15 SCH A 251

Accurate thermodynamic properties of bcc refractories through Direct Upsamling — •Axel Forslund, Jong Hyun Jung, Prashanth Srinivasan, and Blazej Grabowski — Institute for Materials Science, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart

The outstanding high-temperature properties of the bcc refractory elements make them important in many industrial and scientific applications. Accurate thermodynamic data of unary bcc refractories are a requisite, for example, when used as end members for phase diagrams of high entropy alloys. In this work, we have calculated thermodynamic properties of the four bcc refractory elements V, Ta, Mo and W up to the melting point with full DFT accuracy with the newly developed Direct Upsampling method. We present highly converged Gibbs energy surfaces, from which accurate temperature dependence of heat capacity, thermal expansion coefficient and bulk modulus can be derived. We show their convergence with respect to fitting polynomial order and volume-temperature-grid density. Some group trends are observed, related to the electronic densities of states. In our analysis, we also estimate the contribution from thermal vacancies based on a single high-temperature calculation of the vacancy formation free energy. Further, our results are analysed in terms of homologous temperature for the elements of which a theoretical melting point (connected to the specific exchange correlation functional used) is known. The homologous temperature dependence of the calculated properties show a remarkable agreement with experiments.

CPP 48.9 Thu 12:30 SCH A 251

Efficient workflow for treating thermal and zero-point contributions to the formation enthalpies of ionic materials — •Rico Friedrich[1,2,3], Marco Esters[1], Corey Oses[1], Stuart Ki[1], Maxwell J. Brenner[1], David Hicks[1], Michael J. Mehl[1], Cormac Toher[1], and Stefano Curtarolo[1] — [1]Duke University, USA — [2]TU Dresden — [3]Helmholtz-Zentrum Dresden-Rossendorf

The formation enthalpy, quantifying the enthalpy of a compound with respect to its elemental references, is a key parameter for predicting the thermodynamic stability of materials thus enabling data-driven materials design. Although for instance zero-point vibrational and thermal contributions to the formation enthalpy can be quite substantial reaching absolute values of up to ~ 50 meV/atom for ionic systems such as oxides, they are often neglected in *ab initio* workflows.

Here, we first calculate the thermal and zero-point contributions accurately from a quasi-harmonic Debye model. At room temperature, they largely cancel each other due to the different bond stiffness of compound and references reducing the total vibrational contribution to maximally ~ 20 meV/atom [1]. Moreover, the vibrational contributions can be parametrized within the coordination corrected enthalpies (CCE) method completely eliminating the need to compute these terms explicitly. On this basis, using only 0 K *ab initio* data as input, a workflow can be designed providing access to formation enthalpies at different temperatures from the AFLOW-CCE tool [2].

[1] R. Friedrich *et al.*, npj Comput. Mater. **5**, 59 (2019).

[2] R. Friedrich *et al.*, Phys. Rev. Mater. **5**, 043803 (2021).

CPP 48.10 Thu 12:45 SCH A 251

Microstructure-Property Linkages for Effective Elasticity Tensors by Deep Learning — •Bernhard Eidel — TU Freiberg, M5-Micro Mechanics & Multiscale Materials Modeling, Lampadiusstraße 4, 09599 Freiberg

The objective of the present work is to link random heterogeneous, multiphase materials to their elastic macroscale stiffness by 3D convolutional neural networks (CNNs). In an approach of supervised learning the effective elasticity tensors stem from homogenization simulations.

The proposed CNN model is a universal predictor for its extended generalization abilities overcoming bottlenecks in existing studies. It accounts for a large variety of microstructures, for arbitrary phase fractions, for almost arbitrary elastic moduli of the constituent phases, and it predicts the stiffness for periodic boundary conditions (BCs) along with sharp upper and lower bounds for the case of non-periodic matter. The proposed universal CNN model achieves high accuracy in its predictions. For a real, two-phase diamond/SiC coating material the universal CNN is almost as accurate as a CNN exclusively trained for fixed elastic phase properties of that material. The speedup compared to finite element computations for homogenization is above factor 20 500. The proposed CNN model hence enables fast and accurate stiffness predictions in universal analyses of heterogeneous materials in their linear elastic regime, for details see [1].

[1] B. Eidel: Deep CNNs as universal predictors of elasticity tensors in homogenization, Comput. Methods Appl. Mech. Eng. (2023).

CPP 48.11 Thu 13:00 SCH A 251

Influence of doping atoms on twinning in Ni-Mn-Ga alloy: an ab initio study — •Petr Šesták, Martin Hezcko, and Martin Zelený — Brno University of Technology, Brno, Czechia

Magnetic shape memory alloys (MSMAs) are multifunctional materials which - owing to the tight coupling between their magnetic and ferroelastic order - exhibit interesting phenomena, such as giant magnetoresistance, magnetocaloric and elastocaloric effects, and magnetically-induced reorientation (MIR) of martensite. The prototype MSMAs are the Heusler Ni-Mn-Ga based alloys. By combining the large strain and fast response, they may fill the application gap between the shape memory actuators (large strain, slow response) and magnetostrictive/piezo actuators (small strain, fast response). The MSMAs strongly depends on the twinning structure and especially on the twinning stress that is highly dependent on exact alloy composition, as it significantly decreases with increasing content of Mn, which hinders the MIR in Mn-excess alloy.

The recent development in atomistic simulations allows to determine the twinning stress not only from experimental methods but also from theoretical simulations. For example, generalized-planar-fault-energy (GPFE) curves describe the energy pathways associated with twinning as a function of shearing vector. Here, we present results of our calculations to reveal, how doping elements Co, Cu and Fe affects the GPFE curves, and consequently formation and propagation of twins.

CPP 49: 2D Materials VII: Heterostructures (joint session O/CPP)

Time: Thursday 10:30–12:45 Location: GER 37

CPP 49.1 Thu 10:30 GER 37

In-situ growth characterization of 2D heterostructures: $MoSe_2$ on intercalated graphene/Ru(0001) — •Lars Buss[1], Nicolas Braud[2], Moritz Ewert[1], Matteo Jugovac[3], Tevfik Onur Mentes[3], Andrea Locatelli[3], Jens Falta[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Institute for Solid State Physics, University of Bremen, Bremen, Germany — [3]Elettra-Sincrotrone Trieste S.C.p.A, Bazovizza, Trieste, Italy

Despite the great fundamental interest in 2D heterostructures, most of the investigated 2D heterostructures were realized by mechanical exfoliation or chemical vapor deposition in the millibar range, preventing true in-situ characterization of the growth process. Here, we have investigated the growth of $MoSe_2$ on single-layer graphene on Ru(0001) via real-time in-situ low-energy electron microscopy and micro-diffraction. After preparation of the graphene by standard procedures from an ethylene precursor, $MoSe_2$ has been prepared via codeposition of Mo and Se. Prior Se intercalation of the graphene appears to enhance the subsequent growth of $MoSe_2$ on the graphene. At elevated temperatures, rotational ordering of the $MoSe_2$ is facilitated by the strongly enhanced mobility of single-domain $MoSe_2$ islands that align with the high symmetry orientations of the underlying graphene, indicating a non-negligible interaction between the two van-der-Waals materials. Micro-spot angle-resolved photoemission proves the monolayer nature of the as-grown $MoSe_2$ as well as the free-standing character of the Se-intercalated graphene underneath.

CPP 49.2 Thu 10:45 GER 37

Designer quantum states in metal-organic frameworks — •Orlando J Silveira[1], Linghao Yan[1], Shawulienu Kezilebieke[2], Benjamin Alldritt[1], Viliam Vano[1], Ondřej Krejčí[1], Jose Lado[1], Adam S Foster[1,3], and Peter Liljeroth[1] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]University of Jyväskylä, FI-40014 University of Jyväskylä, Finland — [3]Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

Vertical heterostructures have emerged as a promising path to the design of quantum materials with exotic properties. Here, we show that this concept can be also extended to a family of 2D kagome metal-organic frameworks (MOFs) of the family M_2DCA_3, with M= Cu and Ni. The two MOFs have been fabricated either on a graphene/Ir(111) surface or the superconducting substrate $NbSe_2$, and the structural and electronic properties of different phases of both 2D MOFs + substrates were studied through density functional theory (DFT) calculations. Results show that the Cu_2DCA_3 MOF is effectively decoupled from the Ir(111) metallic substrate by the graphene layer, which is important to reveal the topological properties of this family of MOF. Moreover, this study extends the synthesis and electronic tunability of 2D MOFs beyond the metal surfaces to superconducting substrates, which are needed for the development of emerging quantum materials. We show that the Ni_3DCA_2 MOF has a spin density around the Ni atom when synthesized on the $NbSe_2$ substrate due to charge transfer, and this makes a perfect platform to realize topological superconductivity.

CPP 49.3 Thu 11:00 GER 37

Phonon gap supported tunneling and Faraday screening through graphene — •Tobias Wichmann[1,2,3], Keda Jin[1,2,4], Jose Martinez Castro[1,4], Honey Boban[5], Lukasz Plucinski[5], Markus Ternes[1,2,4], F. Stefan Tautz[1,2,3], and Felix Lüpke[1,2] — [1]Peter-Grünberg-Institut (PGI-3), Forschungszentrum Jülich, 52425

Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA) - 52425 Jülich, Fundamentals of Future Information Technology, Germany — [3]Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen, Germany — [4]Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen, Germany — [5]Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich, 52425 Jülich, Germany

Encapsulation of van der Waals materials has proven a vital technique to protect them from degradation and contamination. Usually, metallic encapsulation layers mask the properties of the underlying material when studied in scanning tunneling microscopy. Utilizing the inelastic tunneling phonon gap of graphene, however, enables the unfettered investigation of low energy phenomena (e.g. Kondo effect, Majoranas, etc.) by scanning tunneling spectroscopy, while maintaining the advantages of encapsulated samples. Furthermore, we find that the conductive nature of the graphene encapsulation layer screens the sample from tip-induced electric fields, exemplified by our low-temperature STM examination of encapsulated Fe3GeTe2.

CPP 49.4 Thu 11:15 GER 37

Fermi level tuning of a $MnBi_2Te_4$ monolayer — •Marco Dittmar[1], Philipp Kagerer[1], Celso I. Fornari[1], Simon Müller[1], Sergio L. Morelhão[2], Hendrik Bentmann[1], and Friedrich Reinert[1] — [1]Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany — [2]Instituto de Física, Universidade de São Paulo, Brazil

By breaking time reversal symmetry, introducing magnetic order to topological insulators leads to the opening of a 2D surface state gap at the Dirac point. As a second crucial parameter, tuning the position of the Fermi level inside this gap, enables the observation of exciting new phenomena, such as the quantum anomalous Hall effect (QAHE). Here, we focus on the intrinsic ferromagnetic monolayer of $MnBi_2Te_4$, acting as a magnetic extension of the topological insulator Bi_2Te_3 [1]. We tune the Fermi level position in this compound by preparing a single layer of $MnBi_2Te_4$ on top of the topologically non-trivial p-n-junction of Sb_2Te_3 and Bi_2Te_3 grown by molecular beam epitaxy (MBE) [2]. We will present a study containing structural characterization of the heterostructures by X-ray diffraction and atomic force microscopy, while the electronic structure is assessed by X-ray and angle resolved photoemission spectroscopy.

[1] M. M. Otrokov *et al.*, 2D Mater **4**, 025082 (2017)
[2] P. Kagerer *et al.*, arXiv 2207.14421 (2022)

CPP 49.5 Thu 11:30 GER 37

1D Topological Superconductivity in a van der Waals heterostructure probed by Abrikosov vortices — •Jose Martinez-Castro[1,2], Tobias Wichmann[1,3], Tomáš Samuely[4], Keda Jin[1,2], Oleksander Onufriienko[4], F. Stefan Tautz[1,3,5], Markus Ternes[1,2,3], and Felix Lüpke[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen, Germany. — [3]Jülich Aachen Research Alliance, Fundamentals of Future Information Technology, 52425 Jülich, Germany — [4]Centre of Low Temperature Physics, Faculty of Science, P. J. Safarik University & Institute of Experimental Physics, Slovak Academy of Sciences, Kosice, Slovakia — [5]Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen, Germany

The 2D topological insulator monolayer (ML) WTe_2 is characterized by an insulating interior surrounded by helical 1D edge states. When this material is brought into proximity to the s-wave superconductor $NbSe_2$, the spectroscopic features of the helical edge state remain intact while showing a proximity-induced superconducting gap [1]. However, so far there has been no direct evidence that the observed edge superconductivity is of different nature than that observed away from the edge. Here, by inducing Abrikosov vortices at the boundary between ML WTe_2 and $NbSe_2$, we show that the induced superconductivity in the helical edge is robust against magnetic fields, a strong indication of 1D topological superconductivity.

[1] Lüpke et al., Nat. Phys. 16, 526 (2020)

CPP 49.6 Thu 11:45 GER 37

Density functional theory studies of Anthracene on MoS_2 — •Gérald Kämmerer and Peter Kratzer — Faculty of Physics, University of Duisburg-Essen

Thin layers of MoS_2 are attractive as transparent contacts on organic semiconductors, e.g., oligoacene. As a model for molecules with a delocalized system of π-bonds, we investigate the physisorption of a monolayer of anthracene ($C_{14}H_{10}$) on a MoS_2 single layer using density functional theory. The calculations were carried out with the FHI-Aims code with different functionals. Van der Waals interactions are described by a pairwise potential of the Tkatchenko-Scheffler type or by a many-body dispersion technique. We determine structural properties and can identify the relative position of the molecular HOMO and LUMO (Π and Π^*) orbital concerning the band edges of MoS_2. These results can help find the type of band alignment between MoS_2 and an anthracene molecular crystal, as well as the binding energy of the molecule on the surface. The financial support by DFG within CRC 1242 (*Project B 02*) and computation time on the MagnitUDE supercomputer system are gratefully acknowledged.

CPP 49.7 Thu 12:00 GER 37

Lateral heterostructures of graphene and h-BN with atomic lattice coherence and tunable rotational order — •Haojie Guo[1], Ane Garro-Hernandorena[1], Antonio J. Martínez-Galera[2,3], and José M. Gómez-Rodríguez[1,3,4] — [1]Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]Departamento de Física de Materiales, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [4]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain

In-plane heterostructures of graphene and h-BN exhibit exceptional properties, which are sensitive to the structure of the alternating domains. However, achieving accurate control over their structural properties, while keeping a high perfection of the graphene-h-BN boundaries, still remains a challenge. Here, the growth of lateral heterostructures of graphene and h-BN on Rh(110) surfaces is reported. The choice of the 2D material, grown firstly, determines the structural properties of the whole heterostructure layer, allowing to have control over the rotational order of the domains. The atomic-scale observation of the boundaries demonstrates a perfect lateral matching. Lateral heterostructures floating over an oxygen layer have been successfully obtained, enabling to observe intervalley scattering processes in graphene regions. The high tuning capabilities of these heterostructures suggests their usage as testbeds for fundamental studies.

CPP 49.8 Thu 12:15 GER 37

Relaxation mechanisms for in-plane heterostructures of transition metal dichalcogenide monolayers — •Kai Mehlich[1], Francis H. Davis[3], Thais Chagas[1], Daniela Dombrowski[2], Daniel Weber[1], Catherine Grover[1], Arkady Krasheninnikov[3], and Carsten Busse[1] — [1]Derpartment Physik, Universität Siegen, Walter-Flex-Str. 3, 57072 Siegen — [2]Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [3]Ion Beam Centre, Helmoltz-Zentrum Dresden Rossendorf, Bautzner Landstraße 400, 01328 Dresden

We use sequential epitaxial growth to synthesise in-plane heterostructures of MoS_2 and TaS_2 monolayers on Au(111). Even though the two materials have significantly different lattice constants, STM-measurements show that coherent interconnection of the two materials can be achieved. Defects at the interface such as dislocations are absent. We find this for all interfaces, independent of orientation or the widths of the joined materials. This is at variance with DFT-calculations where we find that the formation of dislocations is energetically favoured, at least until a critical width of the heterostructures. Our growth process can thus lead to a metastable, defect-free interface.

CPP 49.9 Thu 12:30 GER 37

Predicting the Gas Sensing Performance of 2D Materials — •Udo Schwingenschlögl, Vasudeo Babar, Hakkim Vovusha, and Altynbek Murat — King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

We study the potential of material simulations based on first-principles methods to predict gas sensing properties of 2D materials. This emerging class of materials is of particular interest to gas sensing applications due to high surface-to-volume ratios and chemical stability. We discuss results of electron transport calculations within the Landauer-Büttiker formalism and compare the conclusions to analyses in terms of the adsorption energy. Journal References: ACS Appl. Nano Mater. 2, 6076 (2019); J. Phys. Condens. Matter 32, 355602 (2020)

CPP 50: Glasses and Glas Transition II

Time: Thursday 12:15–13:00 Location: ZEU 255

CPP 50.1 Thu 12:15 ZEU 255

Analysis of glass transition for polymer melts using data-driven methods — •Atreyee Banerjee, Hsiao-Ping Hsu, Kurt Kremer, and Oleksandra Kukharenko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Upon cooling, the dynamical properties of most polymer melt slow down exponentially leading to a glassy state without any drastic change in structure. While determining glass transition temperature and understanding the glass transition are important topics of current physical research, the properties in the glassy state are crucial for their general applicability. The conventional ways to calculate glass transition temperature from simulation data of polymer melts rely on the fitting of high- vs. low-temperature branches of macroscopic properties such as volume or density and are sensitive to the choice of parameters. We propose a new data-driven approach based on the information about structural fluctuations in the chains to identify the glass transition temperature. Our data-driven approach utilizes high-resolution details accessible through molecular dynamics simulations and considers the structural information of individual chains. The method was tested for coarse-grained weakly semi-flexible polymer model simulations [1]. It is also applied to the all-atom acrylic polymer simulations with different lengths of side-chain residues.

[1] Atreyee Banerjee, Hsiao-Ping Hsu, Kurt Kremer, and Oleksandra Kukharenko, arXiv:2211.14220 (2022)

CPP 50.2 Thu 12:30 ZEU 255

Roughness Induced Rotational Slowdown near the Colloidal Glass Transition — Beybin Ilhan, Michel Duits, and •Frieder Mugele — University of Twente, Physics of Complex Fluids group

Rotational diffusion of colloidal spheres has been studied rarely, in spite of its importance in the kinetics of many processes involving friction. While for smooth hard spheres, rotational diffusion gets impeded only weakly with increasing volume fraction, the picture changes drastically when surface roughness is introduced. We show this for a system of undeformable all-silica colloidal raspberries, studied with time-resolved 3D Confocal Scanning Laser Microscopy (CSLM).

We find that the strong surface roughness leads to a significantly lower maximum volume fraction, preceded by a broad concentration range in which the rotational Brownian motion changes signature from high-amplitude diffusive to low-amplitude rattling. This strong rotational slowdown occurs at significantly higher concentrations than for the translations, thus presenting a second glass transition.

In the regime where the Mean Squared Angular Displacement (MSAD) is subdiffusive, significant correlations are found between the translational and rotational motions. The drastic rotational slowdown occurs when the particle intersurface distance becomes comparable to the surface roughness amplitude. Concurrently, the number of contacts exceeds a critical value. This picture is supported by observations in a densely packed layer of raspberries at a smooth wall: here significant rotational motions are found while the translations are almost completely frozen.

CPP 50.3 Thu 12:45 ZEU 255

When molecular heterogeneities matter: thermal expansion and relaxation time in polyalcohols — •Martin Tress[1], Jan Gabriel[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Leipzig, Germany — [2]Roskilde University, Roskilde, Denmark

Structural relaxation in liquids is considered to depend directly on the available free volume. Many theoretical concepts of liquid dynamics and the glass transition approximate this molecular quantity using macroscopic density. However, particularly hydrogen (H-) bonding liquids defy proper description by these approaches (e.g. the failure of density-scaling in such materials). To study densification on molecular scale, we use infrared spectroscopy on a series of polyalcohols. By analyzing specific molecular vibrations and correlating them with interatomic bond lengths, the thermal expansion of several types of intramolecular covalent bonds and intermolecular H-bridges is quantified. Pronounced differences between intra- and intermolecular expansion verify the dominance of the latter. Surprisingly, the overall thermal expansion (i.e. cube root of inverse density) is even bigger than that of the strong H-bridges. This suggests that weak H-bridges dominate thermal expansion while strong ones must control structural relaxaztion, i.e. the glass transition. The method is validated by successfully describing the density of water based on extracted H-bridge lengths. Consequently, inhomogeneities on intra- and intermolecular scale can play distinct roles in densification and orientational relaxation and require a careful consideration in a comprehensive theoretical description. [Gabriel, Tress et al. J Chem Phys 154 (2021) 024503]

CPP 51: Hybrid and Perovskite Photovoltaics III

Time: Thursday 15:00–17:15 Location: GÖR 226

CPP 51.1 Thu 15:00 GÖR 226

Slot-die coating of nanocrystal and bulk perovskite thin films for photovoltaics — •Manuel A. Reus[1], Ahmed Krifa[1], David P. Kosbahn[1], Quinten A. Akkerman[2], Alexander Biewald[3], Lennart K. Reb[1], Matthias Schwartzkopf[4], Andrei Chumakov[4], Stephan V. Roth[4], Achim Hartschuh[3], Jochen Feldmann[2], and Peter Müller-Buschbaum[1,5] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching — [2]Nano-Institut München und Fakultät für Physik, LMU München — [3]Department Chemie und CeNS, LMU München — [4]DESY, 22607 Hamburg — [5]MLZ, TUM, Garching

Thin-film solar cells might offer large-scale and cheap production with highly tunable properties, e.g., semi-transparency, color, thickness, or flexibility. Slot-die coated nanocrystal and bulk hybrid perovskite thin films are significant for high-efficiency next-generation solar cell absorber materials. In this work, we show the feasibility of creating high-quality thin films of this material class by the easily scalable and roll-to-roll compatible deposition method of meniscus-guided slot-die coating. We use time-resolved grazing-incidence X-ray scattering to investigate the crystal structure, texture, and morphology of the printed thin films. We track the printing process in real-time and extract parameters describing the quality and kinetics of the printing process. We also present solar cell data with perovskite absorber layers printed from colloidal hybrid perovskite nanocrystal solution.

CPP 51.2 Thu 15:15 GÖR 226

Time-resolved structural changes in hybrid perovskites under illumination — •Ivan Zaluzhnyy[1], Linus Pithan[1], Alexander Hinderhofer[1], Rustam Rysov[2], Fabian Paulus[3], and Frank Schreiber[1] — [1]Institute of applied physics, University of Tübingen, Tübingen, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [3]Center for advancing electronics Dresden, Technical University of Dresden, Dresden, Germany

Hybrid perovskites with mixed halides are known to undergo phase segregation when illuminated by visible light. We used coherent X-ray diffraction at synchrotron sources to reveal the structural changes in the series of $\mathrm{MAPbBr}_{(3-x)}\mathrm{I}_x$ perovskites illuminated with a white and blue light (broad spectrum and $\lambda \approx 450$ nm, respectively). The experimental data allow us to characterize the initial structure of the perovskite films, observe the changes during the illumination, and estimate the time scales over which these changes take place. Moreover, using x-ray photon correlation spectroscopy (XPCS), we can observe the movement of the domain walls and characterize the mobility of the halide ions. The obtained results allow us to better understand the microscopic mechanisms leading to the halide segregation.

CPP 51.3 Thu 15:30 GÖR 226

Investigation of defects inside of mixed halide perovsike solar cells — •Pascal Rohrbeck[1], Yenal Yalcinkaya[1,2], and Stefan A. L. Weber[1,2] — [1]Max Planck Institute for polymer research, department physics at interfaces, Ackermannweg 10, 55128 Mainz, Germany — [2]Johannes Gutenberg University, Department of Physics, Staudingerweg 10, 55128 Mainz, Germany

Understanding the electron and ion dynamics is an important task for improving the lead halide perovskites and related devices. For this task, macroscopic measurement techniques are not sufficient. Therefore, nanoscale characterization methods can play an important role in studying perovskite solar cells. In this study, we investigate the spatial defect distribution in the vicinity of grain boundaries. We introduce local photovoltage, photovoltage decay, and defect mapping via time-resolved Kelvin probe force microscopy (tr-KPFM) methods. We are able to detect and localize areas of increased charge carrier recombination, ion migration, and defects. This will help to understand recombination losses and improve perovskite solar cells on the long run.

CPP 51.4 Thu 15:45 GÖR 226

Post-Flight Analysis of Space-Probed Perovskite and Organic Solar Cells by Means of Grazing-Incidence X-Ray-Scattering — •Lennart Klaus Reb[1], Michael Böhmer[1], Benjamin Predeschly[1], Sebastian Grott[1], Christian Ludwig Weindl[1], Goran Ivkovic Ivandekic[1], Renjun Guo[1], Lukas Viktor Spanier[1], Christoph Dreissigacker[2], Jörg Drescher[2], Roman Gernhäuser[1], Andreas Meyer[2], and Peter Müller-Buschbaum[1,3] — [1]TU München, Garching, DE — [2]Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, DE — [3]Heinz Maier-Leibnitz-Zentrum, Garching, DE

Thin-film perovskite and organic solar cells exhibit an exceptional power per mass that makes them particularly interesting for space applications. Recently, we launched perovskite and organic solar cells into space on a suborbital rocket flight for the first time [1, 2]. The rocket experiment enables post-flight characterization of the space-probed solar cells, based on Grazing-Incidence Small-Angle and Wide-Angle X-ray Scattering (GISAXS/GIWAXS) to investigate morphological and structural changes in the active layers. The morphology is altered slightly by the space flight and environmental conditions before and after the rocket launch; interestingly, the sole solar cell transport in nitrogen environment modified their active layers compared to the reference solar cells. The crystalline phase, however, does not reveal changes in any solar cell type. [1] L. Reb et al., Joule 4,1880-1892 (2020), doi.org/10.1016/j.joule.2020.07.004. [2] L. Reb et al., Rev. Sci. Instrum. 92 (2021), doi.org/10.1063/5.0047346.

CPP 51.5 Thu 16:00 GÖR 226

Simulation of the impact of processing conditions on the perovskite film morphology — •Martin Majewski, Olivier Ronsin, and Jens Harting — Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen- Nürnberg (IEK-11), Dynamics of Complex Fluids and Interfaces, Cauerstraße 1, 91058 Erlangen, Germany

The solution-processed perovskite layer forms complex structures during drying. This morphology of the dry film heavily influences the efficiency of the final solar cell. The impact of the physical mechanisms on the morphology, like for example nucleation and evaporation rate, in a drying, crystallizing wet film is not really understood yet. Therefore a better understanding of the interplay of these phenomena is needed. We will present phase field simulations which are capable to describe the main physical processes like: evaporation, diffusion, spontaneous nucleation, crystal growth and advection, to investigate the impact of processing conditions on the final morphology of the perovskite film. Comparisons of the simulation to the theory will be presented. First simulations of drying solutions, including all physical phenomena, will be shown and compared to experiments.

15 min. break

CPP 51.6 Thu 16:30 GÖR 226

Influence of mesoporous-TiO$_2$ on mobile ion migration and charge extraction of perovskite solar cells — •Patrick Dörflinger[1], Valentin Schmid[1], Yong Ding[2], Mohammad Khaja Nazeeruddin[2], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Group for Molecular Engineering of Functional Materials, Institute of Chemical Sciences and Engineering, EPFL Valais, Sion 1950, Switzerland

Hybrid lead halide perovskite solar cells have reached over 25% power conversion efficiency in the past years but still suffer from poor long term stability. Therefore, increasing attention is given to interfacial engineering. Especially the interplay of the transport layer with the perovskite layer is essential, determining various key properties like the ability of charge extraction or surface recombination. In this study, the potential of different mesoporous TiO$_2$ electron transport layers (ETL) with focus on the mobile ions is investigated. Therfore, concentration and diffusion of mobile ions, often linked to device degradation, is analyzed by measuring open-circuit voltage decay (OCVD). Furthermore, measuring the photoluminescence quenching efficiencies (PLQE) between open-circuit and short-circuit conditions of complete devices allows to study charge extraction and link the obtained results to device performance. These studies prove the advantage of using a mesoporous-TiO$_2$ layer made of single-crystalline nanoparticles as an ETL.

CPP 51.7 Thu 16:45 GÖR 226

Interferometric Bulk Access in Pump-Probe Microspectroscopy of MAPbBr$_3$ Crystals — •Tobias Seewald[1], Ulrich J. Bahnmüller[2], Sebastian Polarz[2], and Lukas Schmidt-Mende[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Institute of Inorganic Chemistry, Leibnitz University Hannover, Germany

We present a microspectroscopic study on individual facets of MAPbBr$_3$ crystals synthesized via an aerosol method controlling the exposed lattice planes. Transient reflection and photoluminescence spectra collected from single few μm facets allow to correlate the findings to micromorphology and lattice termination. Internal reflection of the probe pulse is found to form Fabry-Pérot resonances in the subband gap spectral region, which sensitively respond to the modified refractive index upon photoexcitation. Comparing one- and two-photon pump absorption, the dynamics of bulk and surface states can be distinguished on ps timescales.

CPP 51.8 Thu 17:00 GÖR 226

An alternative non-invasive technique for studying hybrid perovskite solar cells' in-situ degradation — •Chikezie Williams Ugokwe[1,2], Zekarias Teklu Gebremichael[1,2], Kehinde Ogunmoye[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, Philosophenweg 7a, 07743 Jena, Germany — [2]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstrasse 10, 07743 Jena, Germany

The main obstacle to the commercialization of hybrid organic-inorganic perovskite (HOIP) solar cells is stability. Hence understanding degradation routes within the solar cell is essential. Traditional characterization methods have so far either monitored global properties, which precludes a better knowledge of local degradation processes, or induced some type of degradation, which conflates results in in-situ degradation studies of perovskite solar cells. In this paper, we describe a non-invasive technique for the in-situ analysis of the degradation of the active layer of an inverted HOIP solar cell. Utilizing the phenomenon of coherent light propagation in thin film layer stacks, we were able to see lead (II)iodide formation over time in a fully functional perovskite solar cell, which is an undeniable by-product of degradation. We were able to quantify the vertical distribution of the degradation product along the thickness of the active layer by using the measured reflectance of the entire solar cell as the input data for the optical modeling.

CPP 52: Wetting, Fluidics and Liquids at Interfaces and Surfaces III (joint session CPP/DY)

Time: Thursday 15:00–16:15 Location: MER 02

CPP 52.1 Thu 15:00 MER 02

Hierarchical superhydrophobic composite membrane for enhanced distillation with excellent fouling resistance — •Prexa Shah[1], Youmin Hou[2], Michael Kappl[1], and Hans Jürgen Butt[1] — [1]Max-Planck-Institute for Polymer Research, Physics at Interfaces group, Ackermannweg 10, 55128 Mainz, Germany. — [2]School of Power and Mechanical Engineering, Wuhan University, 430072, Wuhan, China.

In arid areas near the coast, seawater desalination has become an essential supply of clean water. As a result, energy-efficient desalination systems must be developed to avoid overburdening the restricted energy supply. Membrane distillation (MD) is gaining popularity as a hybrid thermal/membrane-based desalination approach that may use waste heat for small-scale desalination as well as treating high-salinity brines. The objective is now to maximize the distillation rate while avoiding membrane wetting and fouling. In this work, composite membranes with multiscale pore sizes are formed by depositing a thin layer of nano-porous nanofilaments over microporous membranes. Distillation performance and fouling resistance are explored utilizing low surface tension impurities, which might enhance the chance of membrane wetting. The resistance of protein adsorption to organic fouling is also examined. Our unique multiscale porous membranes outperform traditional hydrophobic membranes in terms of fouling resistance while achieving better distillation flow. This research shows how to optimize MD procedures for wastewater and saltwater treatment.

CPP 52.2 Thu 15:15 MER 02

Surface tension of cavitation bubbles — •Marine Bossert[1], Panayotis Spathis[2], Pierre-Étienne Wolf[2], Laurent Cagnon[2], Isabelle Trimaille[3], and Étienne Rolley[4] — [1]Institut of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Institut Néel, Grenoble, France — [3]Institut des NanoSciences de Paris, Paris, France — [4]Laboratoire de Physique de l'Ècole Normale Supérieure, Paris, France

The evaporation of a fluid contained in a porous material occurs by cavitation when the pores are connected to the outer gas reservoir through small constrictions. Using monolithic transparent porous samples, we have measured the cavitation rate J as a function of the departure from equilibrium for hexane at room temperature [1] and nitrogen over a wide temperature range.

When the radius of the critical nucleus R* is large, our measurements are in agreement with the prediction of the Classical Nucleation Theory. However, when the thickness of the interface is not negligible compared to R*, we find that J is much larger than predicted. We show that this shift can be accounted for if the liquid-vapor surface tension is allowed to depend on the interface curvature. This dependence is in reasonable agreement with Density Functional calculations for Lennard-Jones fluid, including the correction to second order in curvature.

[1] V. Doebele, et al, Phys. Rev. Lett. 125 (2020) 255701.

CPP 52.3 Thu 15:30 MER 02

Simulations for Wetting of Biomembranes — •Marcel Mokbel and Sebastian Aland — TU Bergakademie Freiberg, Freiberg, Germany

The dynamics of membranes, shells, and capsules in fluid flow has become an active research area in computational physics and computational biology. The small thickness of these elastic materials enables their efficient approximation as a hypersurface, which exhibits an elastic response to in-plane bending and out-of-plane stretching deformations. If such a closed thin shell is filled with (and/or surrounded by) multiple fluids, capillary forces on the contact line between the fluids and the shell may arise and force the shell to deform.

In this work, we present a novel Arbitrary Lagrangian-Eulerian (ALE) method to simulate such elastic surfaces immersed in Navier-Stokes fluids, which is combined with a phase field approach to model droplets inside and/or outside the surface. This method combines high accuracy with computational efficiency, since the grid is matched to the elastic surface and can therefore be resolved with relatively few grid points near the surface. We formulate elastic surface forces and propose an evolving finite-element discretization. Several wetting test cases demonstrate the versatility of the proposed method. Examples are simulations of single or multiple droplets deforming a vesicle-like shell.

CPP 52.4 Thu 15:45 MER 02

Dilute suspensions of chemically active particles in thin liquid films — •Tilman Richter, Paolo Malgeretti, and Jens Harting — HELMHOLTZ-INSTITUT ERLANGEN-NÜRNBERG FÜR ERNEUERBARE ENERGIEN, Erlangen, Germany

Thin liquid films are important for many microfluidic applications such as printing or coating of e.g. printable electronics or photovoltaic cells as well as so called lab-on-a-chip devices. Also in catalysis at liquid interfaces thin film dynamics are important. It is well known that a thin film on a solid substrate can be unstable and droplet formation may arise.

The dynamics of thin liquid films and their instability has been the subject of intensive experimental, analytical, and numerical studies, the latter often based on the thin film equation. We propose a set of newly developed equations for the influence of chemical active colloids suspended in a thin liquid film based on the lubrication and Fick-Jackobs approximation. For this novel set of equations we perform a linear stability analysis (LSA) that reveals surprisingly interesting dynamics. We identify the subset of parameters for which the thin film becomes stable i.e. is not rupturing, as well as a variety of different dominating wave-modes. This allows us to control not only the stability but also the droplet size distribution after film rupture, as well as the time it takes for an initially flat film to rupture.

In order to assess the asymptotic state of the thin film, the LSA results are compared against numerical simulations using the Lattice Boltzmann method.

CPP 52.5 Thu 16:00 MER 02

Light properties and water resistant of combined sobrerol methacrylate cellulose thin films. — •Constantin Harder[1,2], Alexandros E. Alexakis[3], Marie Betker[1,3], Yusuf Bulut[1,2], Benedikt Sochor[1], Huaying Zhong[2], Guangjiu Pan[2], Manuel Reus[2], Korneliya Goordeyeva[3], Apostolos Vagias[2,4], Daniel Söderberg[3], Eva Malmström[3], Peter Müller-Buschbaum[2,4], and Stephan V. Roth[1,3] — [1]DESY, 22607 Hamburg, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [3]KTH Royal Institute of Technology, 10044 Stockholm, Sweden — [4]MLZ, TUM, 85748 Garching, Germany

Functionalization of porous materials in terms of optical, chemical and mechanical properties is achieved by applying fully wood-based layers materials. In this project, the refraction index, extinction coefficient and water adhesion properties of cellulose thin films combined with sobrerol methacrylate colloids are investigated together with their topography and morphology. Cellulose nanofibrils (CNF) are a hydrophilic material, and form networks during the drying with specific refraction index, extinction coefficient. Applying additional colloids, their optical properties and water-contact angle can be tuned. Hence, in order to produce water-resistant thin film, a combination of CNF and colloids is a perfect candidate.

CPP 53: Charged Soft Matter, Polyelectrolytes and Ionic Liquid

Time: Thursday 15:00–17:45 Location: ZEU 255

Invited Talk CPP 53.1 Thu 15:00 ZEU 255

Aqueous nanoclusters govern ionic transport in dense polymer membranes — •Joachim Dzubiella — Physikalisches Institut, Universität Freiburg

Hydrated polymer materials with low water uptake exhibit a highly heterogeneous interior characterized by water clusters in the form of nanodroplets and nanochannels. Here, based on our recent insights from computer simulations, we argue that the water cluster structure has large implications for ionic transport and selective permeability in polymer membranes. Importantly, we demonstrate that the two key quantities for transport, the ion diffusion and the solvation free energy inside the polymer, are extremely sensitive to molecular details of the water clusters. In particular, we highlight the significance of water droplet interface potentials and the nature of hopping diffusion through transient water channels. These mechanisms can be harvested and fine-tuned and may optimize selectivity in ionic transport in a wide range of applications.

CPP 53.2 Thu 15:30 ZEU 255

Why weakly hydrated anions bind to polymers but not to monomers? — Bradley A. Rogers[1], Halil I. Okur[1,4], Chuanyu Yan[1], Tinglu Yang[1], •Jan Heyda[2], and Paul S. Cremer[1,3] — [1]Department of Chemistry, The Pennsylvania State University, University Park, PA, USA. — [2]Department of Physical Chemistry, University of Chemistry and Technology, Prague, Dejvice, Czech Republic. — [3]Department of Biochemistry and Molecular Biology, The Pennsylvania State University, University Park, PA, USA. — [4]Present address: Department of Chemistry and National Nanotechnology Research Center (UNAM), Bilkent University, Ankara, Turkey.

Weakly hydrated anions help to solubilize hydrophobic macromolecules in aqueous solutions, but small molecules comprising the same chemical constituents precipitate out when exposed to these ions. Here, this apparent contradiction is resolved by systematically investigating the interactions of NaSCN with polyethylene oxide oligomers and polymers of varying molecular weight. A combination of spectroscopic and computational results reveals that SCN- accumulates near the surface of polymers, but is excluded from monomers. This occurs because SCN- preferentially binds to the centre of macromolecular chains, where the local water hydrogen-bonding network is disrupted. These findings suggest a link between ion-specific effects and theories addressing how hydrophobic hydration is modulated by the size and shape of a hydrophobic entity.

CPP 53.3 Thu 15:45 ZEU 255

Constrained Conductivity in Smallest Polymer Aggregates — •Alaa Hassan, Wing Kit Or, and Martin Tress — Peter Debye Institute, Leipzig university

Detailed insight into material properties at the nanometric level is highly desired in advancing nanotechnology. In the past, Broadband Dielectric Spectroscopy (BDS) revealed altered dynamics of polymers confined to thin films or nanometric channels. However, little is known about the properties of individual polymer chains because of the extreme experimental challenge. We aim to investigate individualized polymer chains using nano-BDS by refining a nanostructured electrode setup and combining it with chemical surface modification. The latter involves depositing a very regular pattern of gold nanoparticles (AuNPs) of well-controllable size and separation at the nanometer scale. These AuNPs act as anchors for chemical grafting-to of thiol-terminated polyethylene oxide (PEO). AFM is used to determine the volume of PEO grafted to each AuNP from which the average number chains are deduced. The successful implementation of this approach is confirmed by measuring the conductivity of separated PEO aggregates down to about five chains each. The conductivity of the isolated aggregates shows Arhinus-like behavior in the whole temperature range, while in bulk, this is only seen below the glass transition. Additionally, the slope of the conductivity in the loss spectra is reduced in the aggregates, which suggests that intra-chain hopping dominates as opposed to inter-chain hopping in bulk. This might exemplify structural constraints that restrict charge mobility close to the surface.

CPP 53.4 Thu 16:00 ZEU 255

KCl modulated D2O Hydration and Subsequent Thermoresponsive Behavior of Poly(sulfobetaine)-Based Diblock Copolymer Thin Films — •Peixi Wang[1], Christina Geiger[1], Julija Reitenbach[1], Apostolos Vagias[5], Robert Cubitt[2], Viet Hildebrand[3], André Laschewsky[3], Christine M. Papadakis[4], and Peter Müller-Buschbaum[1,5] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching — [2]Institut Laue-Langevin, Grenoble — [3]Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm — [4]TUM School of Natural Sciences, Soft Matter Physics, Garching — [5]MLZ, TUM, Garching

The salt effect of KCl on D2O hydration and subsequent thermoresponsive behavior of diblock copolymer (DBC) thin films, which feature a short zwitterionic poly(4-((3-methacrylamidopropyl) dimethylammonio) butane-1-sulfonate)) (PSBP) block and a long nonionic thermoresponsive poly(N-isopropylmethacrylamide) (PNIPMAM) block, is studied by in situ spectral reflectance (SR) and time-of-flight neutron reflectivity (ToF-NR) in combination with isotope sensitivity. The solvation-triggered phase transition upon D2O hydration and subsequent heating is probed in situ by Fourier transform infrared spectroscopy (FT-IR). Besides, the migration and/or aggregation of KCl domains inside the DBC thin films is also demonstrated by complementary methods, namely, X-ray reflectivity (XRR) and atomic force microscopy (AFM).

15 min. break

CPP 53.5 Thu 16:30 ZEU 255

Photoisomerization of Arylazopyrazole Surfactants Drives Property Changes of Polyelectrolyte/Surfactant Mixtures — •Michael Hardt and Björn Braunschweig — University Münster, Center for Soft Nanoscience, 48149 Münster, Germany

Polyelectrolyte/surfactant (P/S) mixtures are in most cases static in nature, which renders them invariable for property changes unless massive changes in pH or ionic strength are applied. We have shown that mixtures of cationic photo-responsive arylazopyrazole (AAP) surfactants with NaPSS exhibit substantial changes in particle size and electrophoretic mobility [1] that can be easily triggered by light irradiation. Here, we present new information on PDADMAC polyelectrolyte mixtures with three anionic AAP surfactants that have H, butyl and octyl terminal groups. The *E* and *Z* configurations of the AAP photoswitches show substantially different hydrophobic interactions that drastically alter their binding affinity to the PDADMAC. Measurements of the electrophoretic mobility clearly indicate that the *E*/*Z* photoisomerization of AAP surfactants causes a charge reversal of the P/S aggregates, while for the H-AAP also larger P/S aggregates in the bulk solution can be dissolved by UV irradiation and formed again with green light. Vibrational sum-frequency generation (SFG) spectroscopy reveals that similar to the changes in the bulk, the charging state at the air-water interface can be reversibly tuned by the light conditions. This has interesting consequences for soft matter materials such as foams [1] and emulsions.

[1] Schnurbus et al., ACS Appl. Mater. Int. 2022, 14, 4656-4667.

CPP 53.6 Thu 16:45 ZEU 255

Grazing incidence x-ray scattering on lithium iron phosphate electrodes with polymer blend binders — •Fabian A.C. Apfelbeck[1], Julian E. Heger[1], Tianfu Guan[1], Matthias Schwartzkopf[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching — [2]DESY, 22607 Hamburg — [3]Royal Institute of Technology KTH, 100 44 Stockholm — [4]MLZ, TU München, 85748 Garching

Lithium iron phosphate (LFP) is a widely used cathode for lithium ion batteries especially in vehicles due to its low cost, high safety, long cycle life and low toxicity. However, so far structural investigations are mainly limited to x-ray diffraction (XRD) techniques. In this project, we extend the investigation of these electrodes to grazing incidence techniques. Therefore, we study electrodes which consist of the active material lithium iron phosphate, carbon black as conducting agent and the polymeric binder polyvinylidenfluorid (PVDF). Additionally, we prepare several binder blends of the neutral PVDF and the single-ion conducting polymer poly(trifluoromethane) sulfonimide lithium styrene) (PSTFSILi) since it is known, that a 1:1 wt%

mixture of PVDF and a single-ion conducting polymer results in superior battery performance. We measure grazing incidence small/wide angle x-ray scattering (GISAXS/GIWAXS) and based on these data, we can understand the influence of the binder on the structure of the electrode. We can correlate ex-situ the morphological and structural data (GISAXS/GIWAXS) with electrochemical results (EIS).

CPP 53.7 Thu 17:00 ZEU 255

Comparative Study of Thermoelectric Transport Properties of Lithium- and Sodium-based Solid Polymer Electrolytes and their Tuning by Carbon-based Additives — •Maximilian Frank, Julian-Steven Schilling, and Jens Pflaum — Experimental Physics VI, University of Würzburg, 97074 Würzburg

Due to the high abundance of their atomic constituents, solution as well as easily scalable processing, and intrinsically low thermal conductivity, organic polymers have gained much attention for potential thermoelectric applications. In particular, ionic systems can generate significantly higher thermal voltages than electronic materials. In this work, we will compare our previous findings [1] on the electrical and thermoelectric transport properties of a solution-processed methacrylate-based solid polymer electrolyte with new results obtained by variation of the conducting salt. Using impedance spectroscopy in a broad frequency range from 100 mHz to 510 kHz in a temperature range between 263 K and 353 K and by means of thermoelectric voltage measurements, we deduced the essential concentration-related differences in the application of LiTFSI and NaTFSI as conducting salts. As an extension, we demonstrate the possibility to efficiently tune the transport properties of these polymer electrolytes by carbon-based additives, which differ in their conductivity characteristics (semiconducting or metallic, 1D or 2D). A proof-of-concept thermoelectric generator verifies the functionality of our approach and substantiates the potential of mixed ionic and electronic materials for future TE applications. [1] M. Frank, J. Pflaum, *Adv. Funct. Mater.* **2022**.

CPP 53.8 Thu 17:15 ZEU 255

Understanding Electron Hopping Mechanism in Organic Radical Batteries — •Souvik Mitra[1], Andreas Heuer[2], and Diddo Diddens[3] — [1]University of Muenster — [2]University of Muenster — [3]University of Muenster

In recent years, there has been an increasing interest in organic radical batteries (ORBs) due to their potentially high power density and availability of Cobalt free cathode materials [1]. Understanding charge transport in ORBs is still an open question due to the disordered behavior of the organic environment [2]. To understand the fundamental mechanism associated with charge hopping and ion transport we use reactive step MD (rs@md) [3]. The rs@md technique accounts for charge transfer reactions in classical MD simulation based on the rates of these reactions. We calculate these rates using the Marcus theory [4]. In this contribution, we explicitly study the Marcus curve for the TEMPO molecule (a very common redox component used in ORBs) in presence of various solvents and salts. We also study the Marcus coupling using quantum methods such as Frontier Molecular Orbital (FMO) [5] and Complete Active Space Self Consistent Field (CASSCF) [6] theories.

[1] Kemper et al., J. Phys. Chem. C 2014, 118, 17213-17220. [2] Kemper et al., J. Phys. Chem. C 2016, 120, 25639-25646. [3] Bidermann et al., J. Chem. Theory Comput. 2021, 17, 2, 1074-1085. [4] Marcus, R.A, J. Chem. Phys. 1956, 24, 5, 966-978. [5] Baumeier et al., Phys. Chem. Chem. Phys., 2010, 12, 36, 11103-11113. [6] Blancafort et al., J. Phys. Chem. C 2006, 110, 20, 6426-6432.

CPP 53.9 Thu 17:30 ZEU 255

Fluid ferroelectric nematic fibres — •Alexander Jarosik and Alexey Eremin — Otto-von-Guericke Universität, Magdeburg, Germany

Nematics with a broken polar symmetry is one of the fascinating recent discoveries in soft matter. High spontaneous polarisation and the fluidity of the ferroelectric nematic NF phase make such materials attractive for future applications and interesting for fundamental research. We report the first example of metastable fluid fibres formed in the ferroelectric phase and characterise their polar and nonlinear optical properties. We discuss the filament stability in the frame of the polarisation-splay model of the ferroelectric nematic phase.

CPP 54: 2D Materials VIII

Time: Thursday 16:30–17:45 Location: MER 02

CPP 54.1 Thu 16:30 MER 02

Structure elucidation of 2D covalent organic frameworks — •Maryke Kouyate[1,3], Konrad Merkel[1], Dominik Pastoetter[2], Albrecht Ludwig Waentig[2], Xinliang Feng[2], and Frank Ortmann[1] — [1]Technical University of Munich, Munich, Germany — [2]TU Dresden, Dresden, Germany — [3]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

We determine the structure of novel 2D framework materials (known as 2D polymers or 2D COFs) that are based on Diquinoxalino[2,3-a:2',3'-c]phenazine (HATNA) vertex units and different linkers (napthalene vs. pyrene). We simulate the unit cell parameters and stacking patterns with density functional theory. The studied COFs were synthesized and experimentally characterized by our collaborators. Our theoretical studies include extensive xyz scans to find the most energetically favorable stacking geometry. With the results of the xyz scans and the appropriate selection of the unit cell, good agreement is obtained with the experimental PXRD patterns, and individual XRD peaks can be assigned to specific in-plane or out-of-plane directions. Moreover, the simulated structures show a clear difference in the packing of the two COFs which are caused by differences in their linker units. This observation is also consistent with the differences in the experimental PXRD patterns. As a result, we can shed light on the actual cell parameters and stacking behavior.

CPP 54.2 Thu 16:45 MER 02

How to calculate electron-hole interaction efficiently in large covalent organic frameworks? — •Konrad Merkel and Frank Ortmann — TU München, School of Natural Sciences

Solving the Bethe-Salpether equation for crystalline materials with many atoms per unit cell, such as covalent organic frameworks, is computationally very expensive and often not feasible. Established tools are usually not suitable for this class of materials because they have enormous memory requirements due to their large basis sets. An elegant solution is to use material-specific, tailored basis sets that allow a complete description with only a handful of basis functions and therefore require only a fraction of the computational resources. In our talk, we present a technique using Wannier functions as a suitable basis and computing Coulomb matrix elements in this basis. The fully parameterized exciton Hamiltonian is then solved using a linear scaling approach that allows efficient computation of spectral quantities such as the exciton DOS for materials with hundreds of atoms per unit cell.

CPP 54.3 Thu 17:00 MER 02

New Paradigm for Gas Sensing by Two-Dimensional Materials — •Udo Schwingenschlögl, Vasudeo Babar, and Sitansh Sharma — King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

The adsorption behavior and electronic transport properties of CO and NH$_3$ molecules on para-C$_3$Si and meta-C$_3$Si monolayers are studied using first-principles calculations and the non-equilibrium Green's function method. The adsorption sites are determined along with their adsorption energies. It turns out that CO and NH$_3$ molecules physisorb on both monolayers. The current-voltage characteristics show that the para-C$_3$Si monolayer can be used to sense CO and NH$_3$ gases with high sensitivity. In contrast to other two-dimensional materials, the sensing mechanism is not based on charge transfer but on the presence of Dirac states and their susceptibility to symmetry-breaking structural distortions. Journal Reference: J. Phys. Chem. C 123, 13104 (2019)

CPP 54.4 Thu 17:15 MER 02

Tunable gas permeation properties through sub-nanometer porous molecular thin carbon nanomembranes — •Vladislav Stroganov[1], Daniel Hüger[1], Tabata Noethel[1], Christof Neumann[1], Monika Kruk[2], Piotr Cyganik[2], and Andrey

Turchanin[1] — [1]Friedrich Schiller University Jena, Jena, Germany — [2]Jagiellonian University, Kraków, Poland

Molecular thin carbon nanomembranes (CNMs) are 1 nm thick nanosheets with sub-nanometer porosity combined with high mechanical and chemical stability. These properties make them promising for the next generation of filtration and gas separation technologies. Here we investigated influence of the structure of molecular precursors on the gas permeation properties of a series of CNMs. The CNMs were synthesized from self-assembled monolayers of biphenyl substituted carboxylic acids on silver substrate $C_6H_5-C_6H_4-(CH_2)_n-COO|Ag$ (n = 2 - 6) via the electron-irradiation induced cross-linking. We study for this homologous sequence of CNMs the permeation of He, D_2 and D_2O vapors as a function of temperature. We demonstrate that even a smallest variation of the number of $-CH_2-$ units leads to a significant change in the permeation which enables the molecular design of these nanomembranes for nanofiltration.

CPP 54.5 Thu 17:30 MER 02

Vapor Adsorption on CNMs studied with Infrared Spectroscopy — •Jakob Kreie, Petr Dementyev, Neita Khayya, and Armin Gölzhäuser — Physics of Supramolecular Systems and Surfaces, Bielefeld University, Germany

Carbon nanomembranes (CNM) are made by electron induced crosslinking of aromatic self-assembled monolayers. Previous studies show that CNM enable rapid transport of water vapor. This may be related to a strong adsorption of water molecules on the CNM surface. A spectroscopic setup for infrared measurements of vapor adsorption on CNMs is designed to investigate the adsorption on the surface under realistic conditions. For this purpose, a reaction chamber in a polarization-modulation infrared reflection absorption spectroscope (PM IRAS) is connected to a vacuum system in order to be able to control the vapor environment.

First measurements are performed with a terphenyl-4-thiol carbon nanomembrane (TPT-CNM). The results show that even low vapor pressures of heavy water are sufficient to achieve strong adsorption on the surface of the TPT-CNM, which indicates a large influence of the surface effects on water transport through the membrane.

CPP 55: Members’ Assembly

Report of the current Speaker team Election of the second deputy speaker Award of the poster Prize of the CPP Division Miscellaneous

Time: Thursday 18:00–19:00 Location: MER 02

All members of the Chemical and Polymer Physics Division are invited to participate.

CPP 56: Focus: Self-Assembly of Plasmonic Nanostructures (joint session CPP/HL)

Organized by Tobias A. F. König and Markus Lippitz

Time: Friday 9:30–12:30 Location: GÖR 226

Invited Talk CPP 56.1 Fri 9:30 GÖR 226

Self-assembled optical metamaterials — •Ullrich Steiner — Adolphe Merkle Institute, Chemin des Verdiers 4, 1700 Fribourg

The self-assembly of block-copolymers gives rise to numerous 2D and 3D morphologies with characteristic pattern sizes on the 10 nm length scale. These polymer structures can be transformed into plasmonic metals to fabricate 2D metasurfaces and 3D metamaterials. These plasmonic replicas have the appropriate structure sizes for the coupling of plasmon resonances to the visible light spectrum, yielding interesting optical materials.

This presentation will review recent progress in manufacturing and studying these materials and highlight interesting current developments.

CPP 56.2 Fri 10:00 GÖR 226

In Situ Monitoring of Self-Assembly and Plasmonic Shifts during the Growth of AgCu Alloy Nanostructures — •Matthias Schwartzkopf[1], André Rothkirch[1], Niko Carstens[2], Thomas Strunskus[2], Franziska C. Löhrer[3], Senlin Xia[3], Volker Körstgens[3], Peter Müller-Buschbaum[3,4], Franz Faupel[2], and Stephan V. Roth[1,5] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]CAU zu Kiel, Kaiserstr.2, 24143 Kiel — [3]TUM, James-Franck-Str. 1, D-85748 Garching — [4]MLZ, Lichtenbergstr. 1, D-85748 Garching — [5]KTH, Teknikringen 56-58,SE-100 44 Stockholm

While magnetron sputtering is a versatile routine method in industry for the deposition of large area metal and alloy coatings, it can be also used for the preparation of functional nanocomposites with e.g. adjustable optical properties [1]. We investigated in real-time the formation of supported silver, copper, and silver-copper-alloy nanoclusters during sputter deposition on poly(methyl methacrylate) by combining in situ surface-sensitive X-ray scattering with optical spectroscopy [2]. While following the transient growth morphologies, we quantify the early stages of phase separation at the nanoscale, track the shifts of surface plasmon resonances, and quantify the growth kinetics of the nanogranular layers at different thresholds. We are able to extract the influence of scaling effects on the nucleation and phase selection and demonstrate a route to tailor accurately the plasmon resonances of nanosized, polymer-supported clusters. [1] Faupel et al., Adv. Eng. Mater. 2010, 12, 12, 1177-1190. [2] Schwartzkopf et al., ACS Appl. Nano Mater. 2022, 5, 3, 3832-3842.

CPP 56.3 Fri 10:15 GÖR 226

What happens to bovine serum albumin in-between two gold nanoparticles and how this biomolecule defines the plasmonic effect? — Nina Tverdokhleb, •Olga Guskova, Ziwei Zhou, Holger Merlitz, and Vladyslav Savchenko — Leibniz-Institut für Polymerforschung Dresden e. V.

In experiments, spherical gold nanoparticles (NPs) covered by bovine serum albumin (BSA) create 1D Au-BSA nanoarrays on a polymer film. The external mechanical strain applied to the film leads to plasmon-coupled circular dichroism (PCCD) enhancement. To explain this phenomenon, we perform all-atom MD simulations of plasmonic nanostructures, representing BSA in-between two gold NPs. The following steps were undertaken: (1) BSA was adsorbed on the gold wall (a model of NP) in implicit water with optimization of its geometry; (2) the second mobile gold wall was approaching adsorbed protein until the distance between NPs reaches the experimentally measured value; (3) mimicking mechanical stretching mentioned above, an external tensile force applied on the second wall has induced the backbone stretching of the initially compressed BSA. This process is accompanied by the crucial growth of BSA dipole moment along the directional deformation, restructuring of the protein secondary structure from helices to coils upon compression (2), the reorientation of the charged amino-acid residues, and subsequent partial back-folding of the secondary structure elements upon stretching (3). We correlate an observed plasmonic effect in the 1D Au-BSA arrays to the changes in dipole moment and chirality of BSA.

CPP 56.4 Fri 10:30 GÖR 226

Uniform and sensitive Raman signal by self-assembled plasmonic nanoparticle gratings — •Sezer Seçkin[1] and Tobias A. F. König[1,2] — [1]Leibniz-Institut für Polymerforschung e.V., Hohe Straße 6, 01069 Dresden — [2]Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, 01062 Dresden

Despite recent advancements in this field, it is still challenging to manufacture SERS substrates that provide high sensitivity and uniformity over large areas. One can overcome this challenge by employing a colloidal approach such as directed self-assembly of plasmonic nanoparticles into ordered structures [König et al. Advanced Functional Materials 31.36 (2021): 2105054]. Here, we have produced highly ordered 1D plasmonic lattice structures by assembling nanoparticles of various sizes. With the help of the low optical loss of colloidal gratings, we studied the enhancement capabilities of the SERS substrates by the excitation of a fluorescent reporter Rhodamine 6G, at different wavelengths. We conducted the polarization-dependent SERS enhancement by exciting colloidal gratings parallel and perpendicular to the polarization of the excitation lasers. Moreover, we studied the effect of the surface plasmon modes on the SERS enhancement at different orientations using the FDTD simulation. The mapping technique visually interpreted the SERS performances of other substrates, which supports the reproducibility and uniformity of the Raman signals over larger areas. Controlling the particle size while keeping the periodicity constant allows us to tune the SERS enhancement factor, which can be helpful for various sensing applications.

CPP 56.5 Fri 10:45 GÖR 226

Investigating Charge Transfers in Colloidal Photonic Crystal Slabs — •Swagato Sarkar[1] and Tobias A. F. König[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Institute of Physical Chemistry, Hohe Str. 6, 01069 Dresden, Germany — [2]Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, Helmholtzstraße 18, 01069 Dresden

The challenges of large-scale and low-loss plasmonic charge transfers are systematically investigated by optical designs with colloidal 1D plasmonic lattice structures. These plasmonic lattices are used as couplers to confine the incident energy into the underlying titanium dioxide layers, thus acting as colloidal photonic crystal (cPhC) slabs. Conventionally, photodetection is possible at energy levels close to the semiconductor bandgap; however, with the observed plasmonic-photonic hybrid modes, the extended solar spectrum can be used for energy harvesting. The photo-amplified current is measured locally with simple two-point contact on the centimeter-sized nanostructure by applying a bias voltage. The optical concepts for metallic grating composed of nanobars are extended for the first time to colloidal self-assembled gold nanoparticle (AuNP) chains to make large-scale charge injection accessible at a reasonable cost. Further, the possibility of photodetection by electric field vectors lying both along and perpendicular to the grating lines can be achieved by tuning the plasmonic grating periodicities.

CPP 56.6 Fri 11:00 GÖR 226

Self-assembled plasmonic metasurfaces for sensing and photocatalysis — •Olha Aftenieva[1] and Tobias A.F. König[1,2] — [1]Leibniz-Institute for Polymer Research Dresden, Hohe Straße 6, 01169 Dresden, Germany — [2]Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, 01062 Dresden, Germany

Self-assembly of colloids allows for robust and tunable manufacturing over centimeter-scaled areas. Here we present the soft lithographic approach for creating plasmonic lattices and demonstrate their usage for sensing applications and photocatalysis. First, a particular case of collective out-of-plane resonant coupling is considered. Such resonances are excited solely under oblique illumination with transverse magnetic polarization and provide field enhancement in the area above the metasurface that is easily accessible to an analyte and is particularly sensitive to the changes in the refractive index. On the other hand, we realize imprinting of such periodic plasmonic lattices on functional substrates, including glass, silicon wafers, carbon, gold, semiconductor, or polymer thin films, illustrating the versatility of the colloidal approach. In particular, the combination of titanium dioxide thin waveguiding layers and plasmonic metasurface gives rise to narrow-bandwidth guided plasmon-polariton modes. Moreover, it induces the generation of hot charge carriers and enhances photocatalytic processes. Thus, colloidal self-assembly of plasmonic metasurfaces presents an application-oriented approach that is of potential use for optical sensors, photonic circuit applications, or hybrid device manufacturing.

15 min. break

Invited Talk CPP 56.7 Fri 11:30 GÖR 226

Simulating quantum systems with plasmonic waveguide arrays — •Stefan Linden — Physikalisches Institut, Universität Bonn, 53115 Bonn

Coupled waveguides provide a powerful platform to simulate the evolution of quantum mechanical tight-binding systems in a classical wave environment. The basis for this is the mathematical equivalence between the time-dependent Schrödinger equation and the paraxial Helmholtz equation. In this presentation, we report on the observation of the Wannier-Stark ladder and Bloch oscillations in arrays of plasmonic waveguides with a propagation constant gradient acting as an effective external potential. Moreover, we show that Floquet engineering is a powerful method to tailor the topological properties of plasmonic waveguide arrays. In this context, we demonstrate that time-periodic modulation of dissipation can restore transport quantization in fast Thouless pumps and report on the observation of the anomalous Floquet topological π-mode at optical frequencies.

Invited Talk CPP 56.8 Fri 12:00 GÖR 226

single molecule detection on a smartphone microscope enabled by DNA origami biosensors — •Philip Tinnefeld — Department of Chemistry and Center for NanoScience, Ludwig-Maximilians-Universität München, Butenandtstr. 5-13, 81377 München, Germany

DNA nanotechnology and especially the DNA origami technique allow well-defined assembly of optically active components and sensing units for novel biosensing approaches. We here demonstrate single-molecule detection on a battery driven smartphone microscope enabled by fluorescence enhancement with DNA origami nanoantennas. As further examples, we show DNA origami membrane sensors for curvature and membrane potentials. Finally, DNA origamis are used for a novel superresolution approach combining graphene energy transfer, pMINFLUX and DNA PAINT that enables nanometric 3D superresolution close to the coverslip.

CPP 57: Complex Fluids and Colloids, Micelles and Vesicles II (joint session CPP/DY)

Time: Friday 9:30–13:00 Location: MER 02

Invited Talk CPP 57.1 Fri 9:30 MER 02

Chiral transport of active and passive colloids — •Anke Lindner[1], Andreas Zöttl[2], Olivia du Roure[1], Eric Clement[1], Francesca Tesser[1], and Guangying Jing[3] — [1]PMMH-ESPCI, 10, rue Vauquelin, 75011 Paris, France — [2]Faculty of Physics, University of Vienna, Kolingasse 14-16, 1090 Wien, Austria — [3]School of Physics, Northwest University, Xi'an, 710127, China

Chirality-induced effects are at the origin of bacterial rheotaxis and particle drift in shear flows. Here we investigate such effects using a combination between experiments and theoretical modeling for two systems: E-coli bacteria and 3D printed micro-particles.

The micro-particles consist of a spherical head and a helical tail of different pitch and handedness. We investigate the chirality-induced reorientation dynamics using microfluidics and observe asymmetric orientation bistability perpendicular to the flow direction. We quantitatively explain our findings through a theoretical model without adjustable parameters considering particle elongation, chirality and head-heaviness, in very good agreement with experiments.

We then present a study of the transport of motile bacteria in shear flows. Experimentally, we obtain with high accuracy and for a large range of flow rates, the spatially resolved velocity and orientation distributions. They are in excellent agreement with the simulations of a kinematic model accounting for stochastic and microhydrodynamic properties and flagella chirality. In contrast to the micro-printed particles Brownian rotational noise plays a crucial role in bacterial rheotactic drift.

CPP 57.2 Fri 10:00 MER 02

Active and driven colloids interacting with vesicles — •Antonio Stocco, Vaibhav Sharma, Florent Fessler, and Carlos Marques — Institut Charles Sadron, CNRS University of Strasbourg

When a colloid is close to a lipid giant vesicle, the interaction between the Brownian particle and the fluctuating soft membrane affects not only the particle motion but also the membrane properties. The membrane may change its shape to accommodate the particle and partial or complete engulfment may occur as a function of the energy of adhesion, membrane tension and bending. Furthermore, the interaction between a micrometric solid particle and a giant vesicle membrane may lead to complex dynamics when the system is driven out of equilibrium. Here, we report our efforts with self-propelled Janus colloids and with bare colloids under optical trapping to mimic complex dynamics such as particle endocytosis, the motion of a self-propelled particle confined to a spherical membrane, or the physics of particle engulfment by a membrane. In a wide range of experimental conditions, we have observed that a self-propelled Janus colloid is able to perform orbital motion around a giant vesicle remaining in a non-engulfment state. Still, the active particle is able to impart a force of the order of 0.01 pN on the vesicle, which is however too small to trigger particle engulfment. By applying external forces in the 1-100 pN range, we were able to observe engulfment of bare and Janus colloids by a giant vesicle.

CPP 57.3 Fri 10:15 MER 02

Universal Casimir interaction and its relevance for colloidal and biophysical systems — •Tanja Schoger[1], Benjamin Spreng[2], Gert-Ludwig Ingold[1], Paulo A. Maia Neto[3], and Serge Reynaud[4] — [1]Universität Augsburg, Germany — [2]University of California at Davis, USA — [3]Universidade Federal do Rio de Janeiro, Brazil — [4]Laboratoire Kastler Brossel, France

Colloidal systems and biophysical interfaces involve electrolytic environments where the Debye screening is extremely efficient. Therefore, it was thought that the interaction induced by electromagnetic fluctuations could not give rise to long-range forces in such systems. It has now been shown and experimentally verified [1] that the contribution to the Casimir force or retarded van der Waals force induced by low-frequency transverse magnetic fluctuations is not screened. There thus exists a contribution to the long-range interaction between two objects in an electrolyte two orders of magnitude larger than previously thought at distances as small as one hundred nanometres.

For two dielectric microspheres in salted water at room temperature, the force becomes universal for sufficiently large distances, in that it depends solely on the geometrical parameters and not on dielectric functions. While in general, a significant numerical effort is required to determine the Casimir interaction [2], we have also derived approximate simple expressions [3] accurate enough for most practical applications. - [1] L. B. Pires et al., Phys. Rev. Res. 3 033037, (2021); [2] B. Spreng et al. J. Chem. Phys. 153, 024115 (2020); [3] T. Schoger et al., Phys. Rev. Lett. 128, 230602 (2022)

CPP 57.4 Fri 10:30 MER 02

Interparticle forces between real cement surfaces across aqueous and non-aqueous solvents — •Simon Becker and Regine von Klitzing — Soft Matter at Interfaces, TU Darmstadt, 64289 Darmstadt, Germany

Concrete and cement are highly abundant construction materials. Therefore, their flow behavior in early stages of processing is of great interest. By using chemical admixtures such as superplasticizers (e.g. polycarboxylate ethers - PCEs) their rheological performance can be enhanced. The rheology is governed by the forces between the particles and the forces between particles and the liquid phase.

The aim of this work is to map the force between cement surfaces across an electrolyte via colloidal probe atomic force microscopy (CP-AFM). Since cement hydrates in aqueous solutions the surface changes with time. The challenge is to disentangle different effects like hydration and roughness of the cement surfaces on the interaction. To prevent hydration of the cement the force measurements are conducted in ethanol solutions. For comparison the force measurements are carried out between two silica particles, between cement and silica as well as between cement and cement.

Furthermore, the time dependence of the cement surface due to hydration in water is mapped using tapping mode AFM. Moreover, the hydration time dependent interparticle force between cement surfaces is investigated in aqueous electrolyte solution with and without PCE to approach application related conditions.

CPP 57.5 Fri 10:45 MER 02

Structure and interaction of surface charged polymeric micelles — Lingsam Tea, Lutz Willner, •Jörg Stellbrink, and Stephan Förster — JCNS-1, Forschungszentrum Jülich, 52425 Jülich, Germany

Soft colloids are ubiquitous in synthetic and biological matter and display macroscopically interesting structural and dynamical properties resulting from its hybrid microscopic structure. We established micelles formed by amphiphilic block copolymers as an easy and elegant model system to tailor colloidal softness [1].

In the present work, we introduce surface charges on n-alkyl-PEO-OH micelles resulting in electrostatic interactions in addition to the inherently present steric repulsion. These charges are precisely implemented by oxidation of only the terminal hydroxy group of the PEO block into a carboxy group. We studied intra- and interparticle structure by SANS over a broad range of concentrations, pH and ionic strength and demonstrate that the micellar form factor remains the same independent of the number of charges. However, in contrast to neutral micelles, the charged micelles typically reveal structure factor contributions even at very dilute concentration, arising from the here dominating long-range electrostatic repulsion. Structure factors in the liquid state are analyzed using competing effective interaction potentials. By increasing the concentration a liquid to crystal transition is observed for all systems, but for charged micelles at a much lower concentration compared to the uncharged micelles.

[1] S. Gupta et al., Nanoscale, 7 (2015) 13924.

CPP 57.6 Fri 11:00 MER 02

Structure and dynamics of concentrated suspensions of PMMA-PDMS core-shell particles — •Joel Diaz Maier, Paul Tümmler, and Joachim Wagner — Institut für Chemie, Universität Rostock, 18051 Rostock, Germany

Sterically stabilized polymer particles with silicone based stabilizers find increasing interest as a novel colloidal model system with hard-sphere interactions. In this contribution, the largely unknown behavior of concentrated suspensions of PMMA-PDMS core-shell particles was investigated over a wide range of volume fractions employing static and dynamic light scattering experiments. Static structure factors extracted from scattered intensities are analyzed using integral equation theory. The wavevector-dependent short-time diffusion of the systems can be accurately described using $\delta\gamma$-expansion, based on interpolated experimental structure factors as a direct input. All investigated structural and dynamical properties closely follow theoretical predictions for hard-sphere systems, proving the suitability of these colloidal particles as an easily accessible model system for hard spheres.

15 min. break

CPP 57.7 Fri 11:30 MER 02

Inverse ISAsomes in biocompatible oils - formulation and characterisation — •Florian Trummer[1], Otto Glatter[2], and Angela Chemelli[2] — [1]Universität Stuttgart, Institut für Physikalische Chemie, Pfaffenwaldring 55, 70569 Stuttgart, Deutschland — [2]Technische Universität Graz, Institut für Anorganische Chemie, Stremayrgasse 9, 8010 Graz, Österreich

In contrast to their more common counterparts in aqueous solutions, inverse ISAsomes (internally self-assembled somes/particles) are formulated as kinetically stabilised dispersions of hydrophilic, lyotropic liquid-crystalline phases in non-polar oils. This contribution reports on their formation in bio-compatible oils and their structural characterisation with Small Angle X-Ray Scattering (SAXS), Dynamic Light Scattering (DLS) and optical microscopy [1]. By using these methods, we were able to demonstrate the presence of inverse hexosomes, inverse micellar cubosomes (Fd3m) and an inverse emulsified microemulsion in squalane with a polyethylene glycol (PEG) alkyl ether as the primary surfactant forming the internal self-assembled phase, which was stabilised by hydrophobised silica nanoparticles. Furthermore, an emulsified L_1-phase and inverse hexosomes were formed in triolein with the triblock-copolymer Pluronic P94 as the primary surfactant. In this case, stabilisation was achieved with a molecular stabiliser of type PEG-dipolyhydroxystearate. Finally, triolein was replaced with olive oil which also led to the successful formation of inverse hexosomes.

[1] Trummer, F., Glatter, O. & Chemelli, A. *Nanomaterials* **12**, 1133 (2022)

CPP 57.8 Fri 11:45 MER 02

Anomalous Screening Behavior of Nanometer-Sized Ions — •Thomas Tilger and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

Natural colloidal dispersions have accompanied mankind in the form of blood or milk ever since. Besides this, artificial systems have gained a significant importance for our daily life during the last decades.

Therefore, it is of special interest to gain an understanding of which interparticle forces govern the stability of colloidal dispersions and how this stability can be tailored. The DLVO theory is a powerful framework to describe these interactions. While this description provides a good agreement with experimental data for small 1:1 electrolytes, larger deviations emerge for ions of higher valency and of larger dimensions. For a detailed examination of these border cases, we directly measure the forces between colloidal silica particles in aqueous electrolyte solutions containing nanometer-sized ions by the colloidal probe AFM (atomic force microscopy) technique.

Two different types of nano-ions were chosen as model systems, Keggin ions (silicotungstic acid, STA, a 1:4 system) and Terpyridine-Nickel-complexes with variable charge. Their electrostatic screening behavior reveals significant deviations between the calculated and measured ionic strengths, which indicates some unexpected phenomena.

CPP 57.9 Fri 12:00 MER 02

Charged, screened-charged and hard-sphere fluids studied by confocal microsopy, analytical theory and simulation. — Sahana Kale, Martin Oettel, and •Hans Joachim Schöpe — Universität Tübingen, Institut für angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

We present a joint experimental and theoretical study investigating the fluid structure in direct and reciprocal space of PMMA particles dispersed in various solvents. Using decaline and CHB alone the structure can be well-described using PB-RMSA-Theory for monodisperse systems. Upon adding TBAB we observe that the surface charge can't be screened entirely. To model the fluid structure we use Monte Carlo simulations for a polydisperse hard core Yukawa System. Thus we get meaningful data for the effective charge and salt concentration. The results indicate behavior that is significantly different from HS. Surprisingly the situation is fundamentally different for particles dispersed in a mixture of decaline and TCE. Here all measured observables follow polydisperse Percus-Yevick theory.

CPP 57.10 Fri 12:15 MER 02

Bicontinuous Microemulsion in Porous Materials — •Margarethe Dahl[1], René Haverkamp[2], Larissa Doll[1], Thomas Hellweg[2], and Stefan Wellert[1] — [1]Institut für Chemie, Technische Universität Berlin, Germany — [2]Physikalische und Biophysikalische Chemie, Universität Bielefeld, Germany

While the bulk phase behavior of microemulsions has been intensively studied, the influence of a geometrical confinement has been widely neglected. Understanding the influence of geometrical restrictions yields both, fundamental insights and importance for applications, e.g. decontamination and enhanced oil recovery. In our study, controlled-pore silica glasses (CPGs) serve as confining matrices for bicontinuous microemulsions. Effects of the pore network and surface chemistry on phase behavior and structure of a model microemulsion are studied by using various CPGs with pore diameter between 75 – 1000 Å and ternary bicontinuous microemulsions (water/octane/$C_{10}E_4$). The naturally hydrophilic surfaces of the CPGs were hydrophobically modified to analyze the influence of the surface polarity. We use imaging techniques (cryo-SEM), small angle scattering (SANS, SAXS) with measurements of the advancing contact angles inside the hydrophilic and hydrophobically modified pores (Washburn approach) to explore the microemulsion phase structure in bulk and inside the pores. In this talk, the results of these combined experiments will be presented and discussed.

CPP 57.11 Fri 12:30 MER 02

Diffusion and thermodiffusion of polymers in mixed solvents — •Daniel Sommermann, Jannik Kantelhardt, and Werner Köhler — Physikalisches Institut, Universität Bayreuth, Germany

We present experiments on diffusion and thermodiffusion of polymers in mixed solvents. So far, most works on thermodiffusion have dealt with binary systems or ternary mixtures of small molecules. Binary samples with polymers in solvents have been studied over both a broad concentration and polymer molar mass range. Only a few very recent experiments measured polymers in a binary solvent. In this work, samples made of polystyrene ($M_w = 4880\,g/mol$), toluene and cyclohexane have been analysed using multi-color optical beam deflection (OBD) and supporting single-color thermal diffusion forced Rayleigh scattering (TDFRS). While binary mixtures are readily characterized by one diffusion and one thermodiffusion coefficient, the number of coefficients increases to four plus two for ternaries. The measured signals show three well separated modes that can be assigned to the thermal diffusivity and the two eigenvalues of the mass diffusion matrix. We are particularly interested in the question, to what extent the dynamics of the large entity, the polymer, is coupled to the solvent-solvent dynamics, both with respect to diffusion and thermodiffusion. A first analysis supports the picture of an effective solvent whose internal dynamics is decoupled from the one of the polymer.

CPP 57.12 Fri 12:45 MER 02

Dynamic susceptibility of magnetic nanoplatelet suspensions — •Margaret Rosenberg[1], Sofia S. Kantorovich[1], and Philip J. Camp[2] — [1]Department of Physics, University of Vienna, Vienna, 1090, Austria — [2]School of Chemistry, The University of Edinburgh, David Brewster Road, Edinburgh EH9 3FJ, UK

Particle anisometry and anisotropy provide valuable control parameters to alter the self-assembly, and thermodynamic, rheological, and phase behaviour, of colloidal suspensions. This work is concerned with the dynamic magnetic susceptibility (DMS) of a ferrofluid with platelet-shaped anisotropic particles, which have a fixed out-of-plane dipole moment providing additional, magnetic anisometry. Such a colloidal suspensions is of particular interest as, above a threshold concentration, it exhibits a ferromagnetic nematic phase. Recent experimental work [1] has shown that the DMS spectrum exhibits multiple dynamical modes, suggesting that there might be clusters of particles with distinct rotational timescales. Using Brownian dynamics simulations, we explore the effects of varying nanoparticle concentration - and therefore microstructure - on the DMS, and explain the gap in relaxation times, and changes in the spectrum, that are observed experimentally.

[1] M. Küster et al., "Magnetic dynamics in suspensions of ferrimagnetic platelets", Journal of Molecular Liquids, Vol. 360, (2022), 119484

CPP 58: Polymer Networks and Elastomers

Time: Friday 9:30–11:30 Location: ZEU 255

Invited Talk CPP 58.1 Fri 9:30 ZEU 255

Studies of polymer thermosets using scattering techniques — •Mats Johansson — Department of Fibre & Polymer Technology, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

Thermoset polymers are complex macromolecular structures where the macroscopic properties depend on several different structural features such as crosslink density, rigidity on a molecular level, and internal secondary bond interactions. The final thermoset structure not only depend on the in-going monomers structure but also how these form the network i.e. the polymerization process. The presentation will describe how a combination of scattering techniques and traditional physical and chemical characterization techniques can reveal new insights on the structure / property relationship for thermoset polymers. It is moreover demonstrated that this approach also can be used to monitor the network formation in-situ i.e. how the structures evolves on a nanoscale during polymerization.

CPP 58.2 Fri 10:00 ZEU 255

Effect of π-π stacking interactions on mechanical properties of lignin-based thermosetting resins — •Iuliana Ribca[1], Benedikt Sochor[2], Marie Betker[1,2], Stephan V. Roth[1,2], Martin Lawoko[1], Michael A. R. Meier[3,4], and Mats Johansson[1] — [1]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden — [2]Deutsches-Elektronen Synchrotron (DESY), Hamburg, Germany — [3]Institute of Organic Chemistry (IOC), Materialwissenschaftliches Zentrum MZE, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [4]Institute of Biological and Chemical Systems-Functional Molecular Systems (IBCS-FMS), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany

The transition towards a more sustainable global carbon economy can be achieved by replacing petroleum-based materials with bio-based alternatives. Lignin is the most abundant aromatic resource in nature and a largely unused by-product of the pulp and paper industry. It is considered a good replacement for fossil-based aromatics. One promising strategy for lignin valorization is to produce thermosetting resins. Further applications of these resins require the understanding of their physicochemical properties. An important role on these properties are playing π-π stacking interactions. Different configurations of π-π stacking interactions are favored between the lignin chains, due to the presence of aromatic rings. In this study, it was investigated the effect of π-π stacking interactions on mechanical properties of lignin-based thermosets by small and wide-angle X-ray scattering methods.

CPP 58.3 Fri 10:15 ZEU 255

Strain hardening of hydrogenated acrylonitrile butadiene rubber — •Christoph Gögelein[1] and Marjan Hemstede - van Urk[2] — [1]Arlanxeo Deutschland GmbH, Kaiser-Wilhelm-Allee 40, 51369 Leverkusen — [2]Arlanxeo Netherlands B.V., Urmonderbaan 24, 6167 RD Geleen, The Netherlands

Therban hydrogenated acrylonitrile butadiene rubber (HNBR) is a specialty elastomer used in the automotive and oil and gas markets. It is well known that HNBR with acrylonitrile (ACN) contents above 39 wt% shows strain-induced crystallization (SIC), caused by the crystallization of alternating ethylene-ACN units (Obrecht, 1986). For HNBR polymers with ACN contents lower than 36 wt%, crystallization occurs in longer ethylene units derived from hydrogenated butadiene sequences (Uschold & Finlay, 1974). Besides these well-established findings, there is an ongoing debate up to which temperature SIC occurs for HNBR (Narynbek Ulu, et al., 2017) (Shaw, 2019). Therefore, crystallization of the polymers was studied, using regular and isothermal differential scanning calorimetry at varying storage times. Furthermore, we investigated strain hardening behavior of HNBR networks with varying ACN contents from room temperature (RT) up to 100 °C, as well as at varying crosslink densities and filler loadings. Our results show that there is a significant strain hardening behavior for HNBR vulcanizates with high ACN content, i.e. for $>$ 39 wt% ACN content. The effect is still observed at 60 °C, but not at 80 °C. Surprisingly, strain hardening doesn't enhance the fatigue lifetime for the samples under investigation.

CPP 58.4 Fri 10:30 ZEU 255

From Cellulose Model Surfaces to Elastic Papers — •Cassia Lux, Sabrina Kerz, and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

Paper is a hierarchical material based on cellulose which allows functionalization on different length scales. The resulting multilateral use is especially crucial with regard to reducing plastic use and waste and replacing it with renewable and biodegradable resources. A novelty in terms of mechanical robustness and controllable fluid mechanics are elastic papers, prepared through the functionalization of the paper fibers with elastomeric particles that concentrate at the fiber-fiber-crossing points. In order to study the particle adsorption, planar cellulose model surfaces are prepared to mimic the surface of a cellulose fiber. The elastomeric core shell particles have a pH-responsive polycation shell, and their adsorption to the negative charged cellulose surface is studied in dependence of e.g. pH-value. The question we adress is how the properties of the cellulose surface and the particles affect the contact area between both, and what effect the adsorption has on the elastic behavior of the particles. A special focus is to resolve the core-shell structure of the particles by Indentation AFM.

CPP 58.5 Fri 10:45 ZEU 255

Structure, phase behavior and mechanical properties of the surface of amphiphilic co-polymer networks — •Kevin Hagmann[1], Nora Fribiczer[2], Sebastian Seiffert[2], Carolin Bunk[3], Frank Böhme[3], and Regine von Klitzing[1] — [1]Institute for Condensed Matter Physics, Technische Universität Darmstadt, D-64289 Darmstadt — [2]Department of Chemistry, Johannes Gutenberg University Mainz, D-55128 Mainz — [3]Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden

The underlying study focuses on the structure, phase separation and mechanics of the surface of amphiphilic co-polymer networks (ACNs).[1] The amphiphilic networks are synthesized from tetrameric star-shaped polymers, combining tetra-poly(ethylene glycol) (hydrophilic) and tetra-poly(ϵ-caprolactone) (hydrophobic) to form a 3D gel network. The topology and near surface structure of the networks are studied with atomic force microscopy (AFM). We put special emphasis on AFM phase imaging under various solvent conditions to identify nanophase separation at the interface. Additionally, we like to present the relation between surface structure and swelling and the resulting mechanical and rheological properties laterally and orthogonally to the gel surface of ACNs. In order to evaluate heterogeneities and phase separation, the mechanical and rheological behavior at the interface of the ACNs will be presented on various length scales (nm - μm). The study shows that the environmental conditions have a strong effect on the gel structure and on nano/microrheological properties. [1] Hagmann et al.; Polymers 2022.

CPP 58.6 Fri 11:00 ZEU 255

A mean field model for reversible networks made of star polymers — •Michael Lang[1], Kiran Suresh Kumar[1,2], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, Hohe Straße 6, 01069 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01069 Dresden, Germany

We extend our recent approach [1] for linear equilibrium polymers with cyclization towards reversible networks made of star polymers. These model systems are particularly suited to test generalizations of the theory that account for the formation of cyclic network defects. Monte-Carlo simulation data and our mean field model demonstrate that the lack of pending loops in networks made by a hetero-complementary coupling of the stars leads to a pronounced shift of the position of the gel point of conventional networks towards lower concentrations. Larger cyclic structures in the networks, on the contrary, can develop a stabilizing effect on the network structure and can cause a reduction of the critical concentration for gelation for a suitable set of system parameters. Remarkably, this leads then to the opposite effect of finite loops as known for conventional irreversible gels.

[1] Lang, M.; Kumar, K. S. Macromolecules 54 (2021) 7021, 10.1021/acs.macromol.1c00718.

CPP 58.7 Fri 11:15 ZEU 255

Thermal Conductivity of Semicrystalline Polymer Networks: Crystallinity or Cross-Linking? — •Manoj Kumar Maurya[1], James Wu[2], Manjesh Kumar Singh[1], and Debashish Mukherji[2] — [1]Department of Mechanical Engineering, Indian Institute of Technology Kanpur, Kanpur, UP 208016, India — [2]Quantum Matter Institute, University of British Columbia, Vancouver, BC V6T 1Z4, Canada

Understanding the heat flow in polymers is at the onset of many developments in designing advanced functional materials. Here, however, amorphous linear polymers usually exhibit a very low thermal conductivity κ, often hindering their broad applications. In this context, two common routes to increase κ are via semicrystallinity and cross-linking. It can therefore be inferred that the combination of these two effects may result in a further increase of κ with respect to the systems where only one of these two effects is important. Using molecular dynamics simulations, we investigate κ in semicrystalline polymer networks. Contrary to a prior understanding, we show that a combination of cross-linking and crystallinity does not always increase κ. Instead, a delicate competition between the lattice periodicity, the cross-linker types, and the bond density dictates the tunability of κ in these complex macromolecular systems. These results are also compared with the existing experiments.

CPP 59: Active Matter V (joint session BP/CPP/DY)

Time: Friday 9:30–12:00 Location: TOE 317

Invited Talk CPP 59.1 Fri 9:30 TOE 317
Experiments on Active Polymer-Like Worms — •Antoine Deblais[1], Daniel Bonn[1], and Sander Woutersen[2] — [1]Van der Waals-Zeeman Institute, Institute of Physics, University of Amsterdam, 1098XH Amsterdam, The Netherlands — [2]Van't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, 1098XH Amsterdam, The Netherlands

We propose a new 'active particle' system in which the particles are in fact polymer-like: the Tubifex tubifex or 'sludge' worm. I will discuss three recent experiments that highlight the richness of this active system. In the first experiment, we perform classical rheology experiments on this entangled polymer-like system. We find that the rheology is qualitatively similar to that of usual polymers, but, quantitatively, the (tunable) activity of the particle changes the flow properties. In a second experiment, we disperse the worm in a quasi-2D aquarium and observe their spontaneous aggregation to compact, highly entangled blobs; a process similar to polymer phase separation, and for which we observe power-law growth kinetics. We find that the phase separation of active polymer-like worms occurs through active motion and coalescence of the phase domains. This leads to a fundamentally different phase-separation mechanism, that may be unique to active polymers. Finally, in the remaining time, I will briefly show that we can efficiently separate by size and activity these living polymers using hydrodynamic chromatography technics.

CPP 59.2 Fri 10:00 TOE 317
Filamentous Cyanobacteria Aggregate at Light Boundaries — •Maximilian Kurjahn[1], Leila Abbaspour[1], Philip Bittihn[1], Ramin Golestanian[1,2], Benoît Mahault[1], and Stefan Karpitschka[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, OX1 3PU, Oxford, UK

Filamentous cyanobacteria are among the oldest, yet still most abundant phototrophic prokaryotes on Earth, fixing vast amounts of atmospheric carbon by photosynthesis. Gliding motility, coupled to photophobic responses (direction reversals in response to light intensity gradients), are believed to drive accumulation in suitable light conditions. Here, we demonstrate that photosensitivity goes beyond simple accumulation: Super-filamentous aggregates, capable of collective mechanical action, form at the boundaries of illuminated regions and may, for instance, contract and detach from the substrate, once grown to a critical mass. We explore how the light pattern, in particular its boundary curvature, impacts aggregation. A minimal model of active rods captures the behavior qualitatively. The ecological impact of such behavior is still unclear, but may enable colonies to escape from saturated habitats by switching to a planktonic state.

CPP 59.3 Fri 10:15 TOE 317
Odd dynamics of living chiral crystals — •Tzer Han Tan[1,2,3,4], Alexander Mietke[4,5], Junang Li[4], Yuchao Chen[4], Hugh Higinbotham[4], Peter Foster[4], Shreyas Gokhale[4], Jorn Dunkel[4], and Nikta Fakhri[4] — [1]MPI-PKS, Dresden, Germany — [2]MPI-CBG, Dresden, Germany — [3]CSBD, Dresden, Germany — [4]MIT, Cambridge, USA — [5]University of Bristol, Bristol, UK

Active crystals are highly ordered structures that emerge from the self-organization of motile objects, and have been widely studied in synthetic and bacterial active matter. Whether persistent crystalline order can emerge in groups of autonomously developing multicellular organisms is currently unknown. Here we show that swimming starfish embryos spontaneously assemble into chiral crystals that span thousands of spinning organisms and persist for tens of hours. Combining experiments, theory and simulations, we demonstrate that the formation, dynamics and dissolution of these living crystals are controlled by the hydrodynamic properties and the natural development of embryos. Remarkably, living chiral crystals exhibit self-sustained chiral oscillations as well as various unconventional deformation response behaviours recently predicted for odd elastic materials. Our results provide direct experimental evidence for how non-reciprocal interactions between autonomous multicellular components may facilitate non-equilibrium phases of chiral active matter.

CPP 59.4 Fri 10:30 TOE 317
Optimal collective durotaxis through active wetting — Macià-Esteve Pallarès[1], Irina Pi-Jaumà[2], Isabela Corina Fortunato[1], Valeria Grazu[3], Manuel Gómez-González[1], Pere Roca-Cusachs[1], Jesus de la Fuente[3], •Ricard Alert[4], Raimon Sunyer[1], Jaume Casademunt[2], and Xavier Trepat[1] — [1]Institute for Bioengineering of Catalonia — [2]University of Barcelona — [3]Instituto de Nanociencia y Materiales de Argón — [4]Max Planck Institute for the Physics of Complex Systems

The directed migration of cell clusters enables morphogenesis, wound healing and collective cancer invasion. Gradients of substrate stiffness are known to direct migration of cell clusters in a process called collective durotaxis, but underlying mechanisms remain unclear. Combining theory and experiments, we reveal a connection between collective durotaxis and the wetting properties of cell clusters. Our experiments show that durotaxis is non-monotonic with substrate stiffness, being optimal at intermediate stiffness. Modeling the cell clusters as active droplets, we explain this non-monotonic durotaxis in terms of a balance between active traction, tissue contractility, and surface tension. Finally, we show that the distribution of cluster displacements has a heavy tail, with infrequent but large cellular hops that contribute to durotactic migration. Our study demonstrates a physical mechanism of collective durotaxis based on the wetting properties of active droplets.

15 min. break

CPP 59.5 Fri 11:00 TOE 317
Chlamydomonas axonemes twist during the beat — •Martin Striegler[1,2], Benjamin M. Friedrich[3], Stefan Diez[1,2,3], and Veikko F. Geyer[1] — [1]B CUBE - Center for Molecular Bioengineering, TU Dresden, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany

Motile cilia are slender cell appendages that drive single cell locomotion and fluid transport across surfaces. The motility of cilia is generated by its inner core, the axoneme, which bends by the activity of dynein motor proteins. Generation of bending requires antagonistic dynein activity on opposing sides of the axoneme. How dyneins are activated antagonistically is unknown. Theoretical models propose dynein regulation by mechanical feedback, which entails structural deformations of the axoneme, but direct experimental evidence is missing. To study axonemal deformations during the beat, we purify and reactivate Chlamydomonas reinhardtii axonemes. Using defocused-high-speed-darkfield microscopy, we resolve the 3D waveforms with nanometer resolution on millisecond timescales. We find that asymmetric waveforms have a non-planar component, which is most pronounced during the recovery stroke. To generate non-planarity within the geometric constraints of the axoneme, twist is thought to be required. Using gold-nano-particles as probes attached to the outside of reactivated axonemes, we, for the first time, measure dynamic twisting deformations in reactivated axonemes. We hypothesize that these deformations are involved in controlling dynein motors generating the axonemal beat.

CPP 59.6 Fri 11:15 TOE 317

Curvotaxis - the effect of curvature on cells and tissue — Lea Hppel, Jan Sischka, and •Axel Voigt — Institute of Scientific Computing, Technische Universität Dresden, Germany

How do cells respond to curvature? Does curvature has an influence on cell shape and movement? What are the consequences for collective behaviour of interacting cells in tissue? We address these questions using a multiphase field model on different curved surfaces and compare the results with experimental data on pillars, in tubes and other surfaces. The results show a significant influence of curvature and the possibility to effectively model the observed phenomena with classical models and additional curvature terms.

CPP 59.7 Fri 11:30 TOE 317

Onset of Homochirality in Cell Monolayers — •Ludwig A. Hoffmann and Luca Giomi — Universiteit Leiden, Leiden, Netherlands

Chirality is a feature of many biological systems and much research has been focused on understanding the origin and implications of this property. Most famously, sugars and amino acids that are found in nature are homochiral, meaning that chiral symmetry is broken and only one of the two possible chiral states is ever observed. Perhaps less well-know, something similar is the case for certain types of cells too. They show chiral behavior and only one of the two possible chiral states is observed in nature. Understanding the origin of cellular chirality and what, if any, use or function it has in tissues and cellular dynamics is still an open problem and subject to much (recent) research. For example, cell chirality has already been shown to play an important role in drosophila morphogenesis.

CPP 59.8 Fri 11:45 TOE 317

Dynamic instability of cytoplasmic compartments — •Melissa Rinaldin[1,2] and Jan Brugués[1,2] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany

Early embryos are the epitome of self-organization. Following the cell cycle oscillator, their internal structure is continuously reorganized into precise patterns at remarkable speeds. For example, the mm-sized egg of the frog Xenopus Laevis divides every 30 minutes into equally-sized cells. Physical processes such as autocatalytic growth, active transport, and reaction-diffusion can allow these embryos to keep up with fast cell cycle times, however, their understanding in early development remains largely elusive. Here, we present recent data from experiments of in vitro cytoplasmic extract obtained from frog eggs and exhibiting cell-free division. We show that the properties of the cell cycle oscillator regulate the pattern of cytoplasmic compartments. Specifically, by perturbing the oscillator, we establish that the interface of cytoplasmic compartments is unstable. We demonstrate that such instability arises from competing waves of autocatalytic microtubule growth, and can generate compartment fusion, strongly affecting the early embryonic pattern formation. Altogether, our results propose that the cell cycle oscillator plays a critical role in partitioning the cytoplasm of early embryos, keeping the dynamic instability of cytoplasmic compartments at bay.

CPP 60: Closing Plenary Talk (joint session BP/CPP)

Time: Friday 12:15–13:00 Location: HSZ 03

Invited Talk CPP 60.1 Fri 12:15 HSZ 03

The physical regulation of brain development — •Kristian Franze — IMP, FAU Erlangen-Nürnberg — Max-Planck-Zentrum für Physik und Medizin, Erlangen — PDN, University of Cambridge

The brain is our most complex organ system. Billions of neurons form an intricate network that regulates all major body functions including thought and emotions. However, the brain is not always that complex. It originally starts off as a simple epithelium, i.e., a single layer of cuboid cells. Axons, which transmit information to other cells over large distances, are only formed during embryonic development. Their immense length - up to several meters in some large animals - comes with severe logistic challenges. For example, how is transport of proteins and genetic information achieved from the nucleus, where the DNA is located, to the axon's distant end? And how does an axon growing through a crowded and dynamic environment know where to turn and where to connect? These questions have captured the imagination of neuroscientists for more than a century. However, despite tremendous progress in molecular biology and imaging technologies, many problems remain unresolved. Combining theory and experiments, we here identified how microtubules, which are polar polymers along which molecular motors transport cargo, orient uniformly along the axon to enable long-range transport, and how mechanical tissue properties regulate axon growth through the developing brain. Our results suggest that chemical and physical signals are integrated by neurons, and that their interaction is crucial for proper brain development and function.