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

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Overview of Invited Talks and Sessions

(Lecture halls H 0106, H 0107, H 0110, and H 0111; Poster C and E)

Invited Talks

CPP 1.1	Mon	9:30–10:00	H 0106	**Customized Cathodes for All-Solid-State Battery Application** — •Torsten Brezesinski
CPP 2.1	Mon	9:30–10:00	H 0107	**Lessons learned from coarse-grained molecular simulations of disordered proteins** — •Arash Nikoubashman
CPP 3.1	Mon	9:30–10:00	H 0110	**Flexibility, connectivity, and topological constraints in polymer crystallization** — •Toshikazu Miyoshi
CPP 6.1	Mon	11:30–12:00	H 0106	**Stretchable, redispersible, recyclable: reversible interfaces for electrically conductive hybrids and composites** — •Tobias Kraus
CPP 13.1	Mon	16:15–16:45	H 0107	**The boson peak in the vibrational spectra of glasses** — •Edan Lerner
CPP 17.1	Tue	9:30–10:00	H 0107	**Dipole-driven Self-assembly and Dynamics in Solutions of Charged Macromolecules** — •Murugappan Muthukumar
CPP 18.1	Tue	9:30–10:00	H 0110	**Via bottom-up synthesis of nanoobjects and nanocomposites towards brain-inspired electronics** — •Alexander Vahl
CPP 22.1	Wed	9:30–10:00	H 0106	**Production of various hybrid bio-based gel ink made of polymer grafted nanocellulose, suitable for 3D printing application** — •Julien R.G. Navarro, Xuehe Jiang, Feras Dalloul, Enguerrand Barba, Benedikt Mietner
CPP 24.1	Wed	9:30–10:00	H 0110	**Thermoresponsive polymers in aqueous environments: insights by atomistic simulations** — •Ester Chiessi
CPP 34.1	Thu	9:30–10:00	H 0106	**Towards AI-assisted analysis of surface and small-angle x-ray and neutron scattering data** — •Marina Ganeva
CPP 35.1	Thu	9:30–10:00	H 0107	**Extraordinarily slippery liquid-repellent surfaces using self-assembled monolayers** — •Robin Ras
CPP 36.8	Thu	11:30–12:00	H 0110	**Digital luminescence: Novel platform for minimalistic photonic applications based on programmable luminescent tags** — •Sebastian Reineke
CPP 37.1	Thu	9:30–10:00	H 0111	**Self-organized protein/polysaccharide nano-assemblies for applications in biomedical and food sciences** — •Aristeidis Papagiannopoulos
CPP 41.1	Thu	11:30–12:00	H 0107	**A multi-scale approach to characterize wetting within a porous medium** — •Maja Rücker, Ryan T. Armstrong, Chenhao Sun, Peyman Mostaghimi, Steffen Berg, Paul Luckham, Apostolos Georgiadis, James E. McClure
CPP 44.1	Thu	15:00–15:30	H 0110	**Colloids and the depletion interaction: multi-phase coexistence of colloidal mixtures** — •Remco Tuinier
CPP 50.1	Fri	9:30–10:00	H 0110	**Condensation on soft substrates** — •Ambre Bouillant, Bruno Andreotti, Jacco H. Snoeijer
CPP 50.6	Fri	11:15–11:45	H 0110	**Of Singularities and Controversies: The Soft Wetting Enigma** — •Stefan Karpitschka
CPP 53.1	Fri	11:30–12:00	H 0107	**A hierarchical fabrication strategy for multi-responsive actuators with structural reconfiguration-assisted self-healing ability** — •Qing Chen

Invited Talks of the joint Symposium SKM Dissertation Prize 2024 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H 1012	**Nonequilibrium dynamics in constrained quantum many-body systems** — •Johannes Feldmeier
SYSD 1.2	Mon	10:00–10:30	H 1012	**Controlled Manipulation of Magnetic Skyrmions: Generation, Motion and Dynamics** — •Lisa-Marie Kern
SYSD 1.3	Mon	10:30–11:00	H 1012	**Interactions within and between cytoskeletal filaments** — •Charlotta Lorenz
SYSD 1.4	Mon	11:00–11:30	H 1012	**Field theories in nonequilibrium statistical mechanics: from molecules to galaxies** — •Michael te Vrugt
SYSD 1.5	Mon	11:30–12:00	H 1012	**Lightwave control of electrons in graphene** — •Tobias Weitz

Invited Talks of the joint Symposium New Trends in Nonequilibrium Physics: Conservation Laws and Nonreciprocal Interactions (SYNP)

See SYNP for the full program of the symposium.

SYNP 1.1	Thu	15:00–15:30	H 0105	**Universality classes of nonequilibrium phase transitions with conservation constraints** — •Walter Zimmermann
SYNP 1.2	Thu	15:30–16:00	H 0105	**The many faces of living chiral crystals** — •Nikta Fakhri
SYNP 1.3	Thu	16:00–16:30	H 0105	**Non-reciprocal pattern formation of conserved fields** — •Fridtjof Brauns, M Cristina Marchetti
SYNP 1.4	Thu	16:45–17:15	H 0105	**Phase transitions and fluctuations of nonreciprocal systems** — •Sarah A.M. Loos
SYNP 1.5	Thu	17:15–17:45	H 0105	**Chiral matters** — •William Irvine

Sessions

CPP 1.1–1.6	Mon	9:30–11:15	H 0106	**Energy Storage and Batteries I**
CPP 2.1–2.12	Mon	9:30–13:00	H 0107	**Modeling and Simulation of Soft Matter I**
CPP 3.1–3.11	Mon	9:30–12:45	H 0110	**Crystallization, Nucleation and Self-Assembly I**
CPP 4.1–4.12	Mon	9:30–12:45	H 0111	**Interfaces and Thin Films**
CPP 5.1–5.12	Mon	9:30–12:45	H 1028	**Active Matter I (joint session BP/CPP/DY)**
CPP 6.1–6.5	Mon	11:30–13:00	H 0106	**Composites and Functional Polymer Hybrids I**
CPP 7.1–7.4	Mon	15:00–16:00	H 0106	**Composites and Functional Polymer Hybrids II**
CPP 8.1–8.4	Mon	15:00–16:00	H 0107	**Polymer and Molecular Dynamics, Friction and Rheology**
CPP 9.1–9.8	Mon	15:00–17:15	H 2032	**Crystallization, Nucleation and Self-Assembly II**
CPP 10.1–10.4	Mon	15:00–16:00	H 0111	**Electrical, Dielectrical and Optical Properties of Thin Films**
CPP 11.1–11.12	Mon	15:00–18:30	BH-N 243	**Active Fluids and Microswimmers (joint session DY/BP/CPP)**
CPP 12.1–12.5	Mon	16:15–17:30	H 0106	**Molecular Electronics and Excited State Properties I**
CPP 13.1–13.5	Mon	16:15–17:45	H 0107	**Glasses and Glass Transition (joint session CPP/DY)**
CPP 14.1–14.6	Mon	16:15–17:45	H 0111	**2D Materials**
CPP 15.1–15.45	Mon	18:00–20:00	Poster C	**Poster I**
CPP 16.1–16.12	Tue	9:30–13:00	H 0106	**Modeling and Simulation of Soft Matter II**
CPP 17.1–17.12	Tue	9:30–13:00	H 0107	**Charged Soft Matter, Polyelectrolytes and Ionic Liquids I**
CPP 18.1–18.12	Tue	9:30–13:00	H 0110	**Organic Electronics and Photovoltaics I**
CPP 19.1–19.12	Tue	9:30–12:45	H 0111	**Energy Storage and Batteries II**
CPP 20.1–20.13	Tue	9:30–13:00	H 1028	**Active Matter II (joint session BP/CPP/DY)**
CPP 21.1–21.42	Tue	18:00–20:00	Poster E	**Poster II**
CPP 22.1–22.6	Wed	9:30–11:15	H 0106	**Gels, Polymer Networks and Elastomers I**
CPP 23.1–23.7	Wed	9:30–11:15	H 0107	**Modeling and Simulation of Soft Matter III**
CPP 24.1–24.6	Wed	9:30–11:15	H 0110	**Responsive and Adaptive Systems I**
CPP 25.1–25.6	Wed	9:30–11:00	H 0111	**Molecular Electronics and Excited State Properties II**
CPP 26.1–26.12	Wed	9:30–13:00	H 1028	**Biomaterials and Biopolymers (joint session BP/CPP)**
CPP 27.1–27.12	Wed	9:30–13:00	BH-N 334	**Active Matter III (joint session DY/BP/CPP)**
CPP 28.1–28.56	Wed	11:30–13:30	Poster C	**Poster III**
CPP 29.1–29.5	Wed	15:00–16:15	H 0106	**Gels, Polymer Networks and Elastomers II**
CPP 30.1–30.11	Wed	15:00–18:00	H 0107	**Charged Soft Matter, Polyelectrolytes and Ionic Liquids II**

CPP 31.1–31.10	Wed	15:00–17:45	H 0110	**Organic Electronics and Photovoltaics II**
CPP 32.1–32.8	Wed	15:00–17:30	MA 141	**Focus Session: Novel Approaches to Surface Plasmon Generated Charges and Heat for Photocatalysis I (joint session O/CPP)**
CPP 33.1–33.6	Wed	16:30–18:00	H 0106	**Hybrid and Perovskite Photovoltaics I**
CPP 34.1–34.12	Thu	9:30–13:00	H 0106	**Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods I**
CPP 35.1–35.5	Thu	9:30–11:00	H 0107	**Focus Session: Wetting on Adaptive Substrates I (joint session CPP/DY/O)**
CPP 36.1–36.12	Thu	9:30–13:00	H 0110	**Organic Electronics and Photovoltaics III**
CPP 37.1–37.12	Thu	9:30–13:00	H 0111	**Biopolymers, Biomaterials and Bioinspired Functional Materials (joint session CPP/BP)**
CPP 38.1–38.11	Thu	9:30–13:00	BH-N 334	**Active Matter IV (joint session DY/BP/CPP)**
CPP 39.1–39.8	Thu	10:30–13:00	MA 004	**Focus Session: Ultrafast Processes in Organic Semiconductors and Perovskites I (joint session O/CPP)**
CPP 40.1–40.10	Thu	10:30–13:15	MA 141	**Focus Session: Novel Approaches to Surface Plasmon Generated Charges and Heat for Photocatalysis II (joint session O/CPP)**
CPP 41.1–41.5	Thu	11:30–13:00	H 0107	**Focus Session: Wetting on Adaptive Substrates II (joint session CPP/DY/O)**
CPP 42.1–42.7	Thu	15:00–16:45	H 0106	**Gels, Polymer Networks and Elastomers III**
CPP 43.1–43.8	Thu	15:00–17:30	H 0107	**Wetting, Fluidics and Liquids at Interfaces and Surfaces (joint session CPP/DY)**
CPP 44.1–44.8	Thu	15:00–17:45	H 0110	**Complex Fluids, Colloids, Micelles and Vesicles (joint session CPP/DY)**
CPP 45.1–45.6	Thu	15:00–16:30	H 0111	**Modeling and Simulation of Soft Matter IV**
CPP 46.1–46.11	Thu	15:00–18:00	MA 004	**Focus Session: Ultrafast Processes in Organic Semiconductors and Perovskites II (joint session O/CPP)**
CPP 47.1–47.10	Thu	15:00–17:45	BH-N 334	**Wetting, Droplets, and Microfluidics (joint session DY/CPP)**
CPP 48	Thu	18:00–19:00	H 0110	**Members' Assembly**
CPP 49.1–49.5	Fri	9:30–10:45	H 0107	**Organic Electronics and Photovoltaics IV**
CPP 50.1–50.10	Fri	9:30–12:45	H 0110	**Focus Session: Wetting on Adaptive Substrates III (joint session CPP/DY/O)**
CPP 51.1–51.10	Fri	9:30–12:15	BH-N 243	**Complex Fluids and Soft Matter (joint session DY/CPP)**
CPP 52.1–52.5	Fri	10:30–11:45	MA 004	**Focus Session: Ultrafast Processes in Organic Semiconductors and Perovskites III (joint session O/CPP)**
CPP 53.1–53.5	Fri	11:30–13:00	H 0107	**Responsive and Adaptive Systems II**
CPP 54.1–54.1	Fri	13:15–14:00	H 0104	**Closing Talk (joint session BP/CPP/DY)**

Members' Assembly of the Chemical and Polymer Physics Division

Thursday 18:00–19:00 H 0110

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

CPP 1: Energy Storage and Batteries I

Time: Monday 9:30–11:15 Location: H 0106

Invited Talk CPP 1.1 Mon 9:30 H 0106

Customized Cathodes for All-Solid-State Battery Application — •Torsten Brezesinski — Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Quasi- and all-solid-state batteries are receiving much attention as enabling technologies for next-generation electrochemical energy storage. Similar to conventional Li-ion batteries, high-capacity, layered transition-metal oxides are being considered for use at the positive electrode in combination with superionic thiophosphate (sulfide) solid electrolytes. Yet, such composite cathodes suffer from degradation issues, such as (electro)chemical side reactions and/or particle fracture/pulverization, limiting their utilization. In this presentation, I will highlight the importance of tailoring layered Ni-rich oxides (regarding particle size, composition etc.) for increasing cycling performance of pelletized and slurry-cast electrodes. In addition, I will show data on the effect of protective nanocoatings on interfacial side reactions in solid-state battery cells using argyrodite Li6PS5Cl as ion conductor.

CPP 1.2 Mon 10:00 H 0106

Real-time monitoring of electrochemical reactions in all-solid-state lithium batteries by simultaneous grazing-Incidence small-angle/wide-angle X-ray scattering — •Yuxin Liang[1], Tianle Zheng[1], Kun Sun[1], Fabian A.C. Apfelbeck[1], Ian Sharp[2], Yajun Cheng[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]WSI, TUM, Garching, Germany — [3]NIMTE, Chinese Academic of Sciences, Ningbo, China — [4]DESY, Hamburg, Germany — [5]KTH Royal Institute of Technology, Stockholm, Sweden — [6]MLZ, TUM, Garching, Germany

Polyethylene oxide (PEO)-based composite electrolytes (PCEs) are promising for lithium batteries due to its high safety. However, the material suffers from low conductivity, inhibiting its commercialization. Therefore, it is crucial to understand the electrochemcial process in PCE-based batteries. Using operando grazing-incidence small-angle and wide-angle X-ray scattering, we find that the electrochemical reaction is highly correlated with the buried morphology and crystalline structure of the PCE. The PEO-Li+ reduction and TFSI- decomposition cause changes in both the crystalline structure and morphology. In addition, the reversible Li diffusion process alters the inner morphology, rather than causing structure changes. This work provides a new path to monitor a working battery, thereby enabling detailed understanding of electrochemically-induced changes, which is essential for developing interface stable lithium batteries.

CPP 1.3 Mon 10:15 H 0106

Introducing the LECA package for machine-learning guided optimization of the ionic conductivity — •Mirko Fischer[1], Harrison Martin[1], Peng Yan[2], Christian Wölke[2], Anand Narayanan Krishnamoorthy[2], Isidora Cekic-Laskovic[2], Diddo Diddens[2], and Andreas Heuer[1] — [1]Institute of Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster — [2]Helmholtz-Institute Münster (IEK-12), Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster

We present the Liquid Electrolyte Composition Analysis (LECA) package as a versatile tool, which implements a simplified and semi-automatic workflow for data-driven and machine-learning guided analysis of large data sets, particularly designed for but not limited to High-Throughput-Experiments (HTE). The LECA package combines popular python-based libraries like scikit-learn, Mapie and GPyOpt to enable fast parallel training, hyperparameter-optimization, model comparison, and uncertainty calculation for various regression models. An active learning approach to reduce the amount of data needed to fit a model with high accuracy is under current development and testing.

We demonstrate the performance of the LECA package on a large HTE dataset for the ionic conductivity as an important bulk property of liquid electrolytes with over 200 individual compositions measured, including the organic electrolytes EC, EMC, and PC, and the lithium salts LiPF6 and LiFSI. Furthermore, we show how the LECA package can be used to optimize the ionic conductivity and discover new compositions.

CPP 1.4 Mon 10:30 H 0106

Structural engineering of two-dimensional nanosheets for sodium-ion storage — •Yuhua Chen, Yulian Dong, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Rechargeable sodium-ion batteries (SIBs), with their low cost and abundant Na reserves, have been promising candidates for energy storage and conversion. Among all cathode materials for SIBs, two-dimensional (2D) VOPO4 show high energy storage potential owing to their high working voltage, stable structure, and diverse structure. Nevertheless, the electrochemical performance of VOPO4 is hindered by many factors such as poor conductivity and limited intrinsic interlayer distance. Rational design and structural engineering of 2D nanosheets by intercalation chemistry, such as cationic intercalation, conductive polymer introduction, and atomic doping, tuning their physical and chemical properties, effectively enhances the storage of sodium in thin 2D nanosheets. Here, we explore intercalation chemistry for the storage of Na+ ions in layered VOPO4 hydrates, delivering a high average operating voltage of approximately 3.5 V. The introduction of Fe3+ ions result in a noteworthy increase in specific capacity, reaching 85 mAh g*1 at 0.1 C, which exhibits a commendable capacity retention rate of 62% over 50 cycles. This investigation underscores the substantial impact of Fe3+ doping on the electrochemical performance of VOPO4*2H2O nanosheets, positioning them as promising candidates for high energy density SIBs.

CPP 1.5 Mon 10:45 H 0106

Operando neutron diffraction experiments in order to investigate the lithiation and ageing mechanism of industrial scale multi-layer 5 Ah pouch cells — •Thien An Pham[1,3], Stefan Seidlmayer[1], Ivana Pivarnikova[1,3], Sven Friedrich[4], Alessandro Sommer[5], Christophe Didier[2], Andreas Jossen[4], Rüdiger Daub[5], Vanessa Peterson[2], Peter Müller-Buschbaum[1,3], and Ralph Gilles[1] — [1]TUM, MLZ, 85748 Garching, Germany — [2]ANSTO, Lucas Heights, Australia — [3]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [4]TUM School of Engineering and Design, Chair of Electrical Energy Storage Technology , 80333 Munich, Germany — [5]TUM School of Engineering and Design, Institute for Machine Tools and Industrial Management, 85748 Garching, Germany

The demands for Li ion batteries are increasing and the improvement of battery performances remains one of the main goals of the research. Currently, switching to materials offering higher materials is one approach to achieve higher capacities. Here, the lithiation mechanism and ageing behaviour of silicon anodes and LiNi0.8Co0.15Al0.05O2 (NCA) cathodes in multi-layer 5 Ah pouch cells were studied with neutron diffraction. The batteries were fabricated on a research production line in order to replicate the conditions of commercial cells as close as possible. Uncylced cells were compared to an aged cell at a state of health of 60 percent. Due to ageing, the capacity is decreased, which can be seen in the evolution of the cell parameters of NCA. During relaxation the NCA peaks are shifting indicating structure changes.

CPP 1.6 Mon 11:00 H 0106

Ionic polymer electrolyte for aluminium batteries — •Amir Mohammad, Thomas Köhler, Shuvrodev Biswas, Hartmut Stöcker, and Dirk C. Meyer — Institute of Experimental Physics, TU Bergakademie Freiberg, Germany

Rechargeable aluminium batteries are considered a promising alternative to lithium-based energy storage systems, but their widespread use is hindered by challenges in the electrolyte system, such as leakage and corrosion. This necessitates the use of expensive metal foils (e.g. Mo, Ta, W) as current collectors on the cathode side. However, a new ionic polymer electrolyte has been developed that offers significant improvements in performance, safety, and cost efficiency. The manufacturing process involves the complexation of polyamide-6 (PA6) with aluminium chloride ($AlCl_3$) and the organic salt triethylamine hydrochloride (Et_3NHCl), allowing for the dissolution of up to 20 % PA6 in the sample.

This results in good mechanical properties and a stable electrode-electrolyte interface without compromising the cell performance. The ionic polymer electrolyte does not require separators, has a high ionic conductivity of up to 0.3 mScm^{-1}, and can effectively dissolve and deposit aluminium electrochemically. This innovation has the potential to replace expensive metal current collectors by affordable aluminium foils with protective coatings. The solid ionic polymer presented here is a promising and robust strategy for the development of stable, safe, flexible, and yet inexpensive aluminium batteries.

CPP 2: Modeling and Simulation of Soft Matter I

Time: Monday 9:30–13:00 Location: H 0107

Invited Talk CPP 2.1 Mon 9:30 H 0107

Lessons learned from coarse-grained molecular simulations of disordered proteins — •Arash Nikoubashman — Leibniz-Institut für Polymerforschung Dresden, Deutschland — Technische Universität Dresden, Deutschland — Cluster of Excellence Physics of Life, Deutschland

The discovery of intrinsically disordered proteins (IDPs) has heralded a paradigm shift in molecular biology away from the principle of ”form follows function”. These IDPs can form biomolecular condensates that fulfill numerous functions in living cells, e.g., signal transduction, stress response and controlled reactions. Due to the conceptual similarities between IDPs and classical polymers, physics-based theories and computer simulations can help to understand, predict and engineer the static and dynamic properties of naturally occurring and synthetic IDPs. In this talk, we will present some of the insights we have gained from coarse-grained molecular simulations, and discuss some of the intricacies and limitations of the underlying models. Key findings include that IDPs inherently exhibit heterogeneous interactions that are weak and distributed along the chain contour, and that IDPs collapse at the condensate-water interface and are tangentially oriented.

CPP 2.2 Mon 10:00 H 0107

Phase-Behaviour of Polymer Grafted Colloidal Nano-Crystals with Variable Grafting Density — •William Fall and Henricus Wensink — Laboratoire de Physique des Solides UMR 8502, CNRS, Université Paris-Saclay, 91405, Orsay, France

The effect of short chain grafting on the liquid crystalline ordering of colloidal nano-crystals is investigated using molecular dynamics simulations. Nano-rods with aspect ratios of typical of cellulose nanocrystals (CNCs) are grafted randomly with short oligomers at 5 different grafting densities. Each system is crystallised from the isotropic phase in solution and slowly compressed until the nano-rods spontaneously order. The liquid crystalline behaviour depends strongly on the grafting density as the effective shape and softness of the nanorods is modified. Ungrafted rods exhibit complex biaxial Nematic and Smectic-C phases at very low volume fractions, which are then preserved upon grafting with at least a 50% occupation of surface sites with oligomers, forming a Nematic and a tilted Smectic-I phase. Heavier grafting results in the disappearance of the Nematic phase and a direct transition to a complex Smectic-B. Interesting behaviour is observed at extremely low grafting densities, around 25%, with the disappearance of Smectic phases and a persistent Nematic phase induced by patchy grafting, which transitions to a Lamellar phase at high concentration. Such systems fall outside of the traditional hard or soft rod descriptions of phase-transitions in rod-like LC systems. Our findings point to as yet undiscovered LC behaviour in grafted and ungrafted rod-like nanocrystals.

CPP 2.3 Mon 10:15 H 0107

Mesoscopic modeling of dynamically helical polymers — Keerti Chauhan[1], Maurice Schmitt[2], 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

Synthetic helical polymers are interesting for applications including catalysis, chirality recognition, and templating assembly of functional molecules. Some of these polymers, exhibit dynamic helicity: their conformations can randomly switch between left- and right-handed helical senses because of moderate inversion barriers. The helicity of dynamical polymers can be controlled by ”doping” their chain with small chiral groups. So far, the influence of biasing groups on helicity has been investigated on the basis of 1D Ising models, which have explained cooperative effects such as majority rules and sergeants-and-soldiers behavior. However 1D Ising models cannot describe the structure of a polymer in three dimensional space. Therefore we develop a mesoscopic molecular model for dynamical helical polymers, combining a worm-like chain representation with special chiral potentials [1]. We investigate conformational properties of helical polymers in dilute solutions with emphasis on topology.

[1] Y. Zhao, J. Rothörl, P. Besenius, P. Virnau, and K. Ch. Daoulas, ACS Macro Lett. 12, 234 (2023)

CPP 2.4 Mon 10:30 H 0107

Knots in polymer melts and films — •Maurice Schmitt[1], Sarah Wettermann[1], Hendrik Meyer[2], and Peter Virnau[1] — [1]Johannes Gutenberg-Universität, Institut für Physik, Mainz, Germany — [2]Université de Strasbourg, Institut Charles Sadron, Strasbourg, France

Flory’s hypothesis states that chains in polymer melts can be mapped onto corresponding random walks with characteristic Kuhn lengths and monomer numbers. However, when topological properties, namely knotting probabilities and knot spectra, are considered as measures for chain configurations, corresponding random walks only provide a poor description of chains in the melt, particularly for flexible chains. On the other hand, good agreement between chains in a melt and theta-chains, i.e., single chains at the transition point between a self-avoiding and a globular phase, can be observed with respect to topology. Here, we extend our previous analysis and provide a comprehensive comparison between theta-chains and chains in polymer melts as a function of chain stiffness. Furthermore, we investigate knotting in polymer films with varying thickness and compare their topologies with those of confined theta chains. Knotting probabilities of chains in thin films and confined single chains increase near the boundary of the confinement as chains take up flat conformations with overall decreased radii of gyration.

CPP 2.5 Mon 10:45 H 0107

Model-Based Approach to Reinforcement in Filled and Strain-Crystallizing Elastomer Networks — •Lena Tarrach and Reinhard Hentschke — Bergische Universität Wuppertal, Wuppertal, Deutschland

The objective of this work is the investigation of the interplay and the differences between reinforcement by filler and by strain-induced crystallization (SIC) in elastomer networks such as Natural Rubber. For this purpose, the model for SIC proposed by Plagge & Hentschke [1] is combined with the model for filled rubber developed by Viktorova et al. [2]. The model is extended to investigate the rupture behavior. First, the stress-stretch behavior and crystallinity-stretch curves of non-breaking model networks with variable filler content are analyzed and compared to experimental observations. Secondly, the rupture behavior is examined dependent on the filler content.

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

[2] Viktorova, M. et al. Mesoscopic Model for the Simulation of Dynamic Mechanical Properties of Filled Elastomers: Model Construction and Parameterization. ACS Applied Polymer Materials 2, 5521-5532. https://doi.org/10. 1021/acsapm.0c00868 (2020).

CPP 2.6 Mon 11:00 H 0107

Transferable Local Density-Dependent Friction in tert-Butanol/Water Mixtures — •Moritz Mathes, Viktor Klippenstein, and Nico van der Vegt — TU Darmstadt, Germany

Coarse-grained (CG) models in molecular dynamics (MD) simulations allow to represent the structure of an underlying all-atom (AA) model by deriving an effective interaction potential. However, this leads to a speed-up in dynamics due to the lost friction, which is especially pronounced in CG implicit solvent models. Adding a thermostat based on the Langevin equation (LE) allows to represent the long-time dynamics of CG particles by reintroducing friction to the system. To improve the representability in CG models of heterogenous molecular mixtures and their transferability over the mixture compositions, we parametrise a LE thermostat, where the friction coefficient depends on the local particle density (LD). We simulated *tert*-butanol/water mixtures over a range of compositions, which show distinct clustering behaviour. For these systems we parametrised three different CG models with: 1. no thermostat friction (CG-MD), 2. fixed friction (CG-LE), and 3. local density-dependent friction (CG-LD). The thermostat friction was iteratively optimised with a Markovian variant of the recently introduced *Iterative Optimization of Memory Kernels* (IOMK) method [1]. We find that the CG-LD model reproduces the AA diffusion coefficients well over the full range of mixtures and is therefore transferable. In addition, I will discuss the role of conservative interactions on dynamics and remaining representability challenges beyond diffusion.

[1] J. Chem. Theory Comput. 2023, 19, 1099-1110

15 min. break

CPP 2.7 Mon 11:30 H 0107

Topological phonon boundary modes in polymer chains and supramolecular lattices — •Jose D. Cojal Gonzalez[2,4], Jakub Rondomaski[3,4], Konrad Polthier[3,4], Jürgen P. Rabe[2,4], and Carlos-Andres Palma[1,2,4] — [1]Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, P. R. China — [2]Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [3]Department of Mathematics and Computer Science, Freie Universität Berlin, 14195 Berlin, Germany — [4]Matters of Activity - Image Space Material, Humboldt-Universität zu Berlin, 10178 Berlin, Germany

In the domain of topological band theory, phonon boundary modes with non-trivial topology present desirable properties for atomically-precise technologies, including robustness against defects, waveguiding, and one-way transport. Topological phonon properties remain to be studied both theoretically and experimentally in low-dimensional materials at the atomistic level, such as polymer chains and self-assembled supramolecular lattices, especially under thermal fluctuations. Here we show by means of molecular simulations that these materials, following modified Su-Schrieffer-Heeger (SSH) phonon models with heavy boundaries, exhibit robust topological phonon boundary modes under thermal fluctuations. These modes propagate upon the excitation of a single molecule, in contrast to free boundary modes. Our work introduces the study of topological vibrations in supramolecular systems and suggests potential applications in realizing Hall effect phonon analogues at the molecular scale.

CPP 2.8 Mon 11:45 H 0107

Statistical Analysis of the Dimerization of Amyloid-β(1-40) and Amyloid-β(1-42) — •Christian Lauer and Wolfgang Paul — Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

We present a numerical investigation of the dimerization of the Amyloid-β(1-40) and Amyloid-β(1-42) peptides. The study employs the PRIME20 intermediate resolution protein model and a flat-histogram type Monte Carlo simulation approach that gives access to the thermodynamic equilibrium of the system over the complete control parameter range, which here is the temperature. Thermodynamic analysis reveals that for densities comparable to typical in-vitro experimental conditions, the folding and aggregation transitions of the systems occure simultaneously. However, looking at the difference of intra- and inter-molecular energy contributions, an increased aggregation propensity of Amyloid-β(1-42) compared to Amyloid-β(1-40) is revealed. Hydrogen-bond probability maps show segments at the N-terminus of the peptide with intra-chain anti-parallel alignment, corresponding to intra-chain beta-sheet structures, while the C-terminus shows a more diverse cast of possible configurations. We use Ramachandran plots to further investigate the influence of the different chain segments on the structure formation of Amyloid-β.

CPP 2.9 Mon 12:00 H 0107

Charge and shape anisotropy effects on the phase diagram of BSA in a coarse-grained model — •Jens Weimar, Frank Hirschmann, and Martin Oettel — Eberhad Karls Universität Tübingen, Germany

Bovine Serum Albumin (BSA) is a model globular protein in biophysical research. However, since it consists of more than 500 amino acid residues it is computationally not yet feasible to perform an all-atom simulation of a system containing many BSA molecules. Hence, we employ an existing low resolution 6-bead coarse-grained model with van der Waals and electrostatic interactions between beads and use grand canonical simulations to determine its phase diagram. At the isoelectric point, different charges on the beads define a charge anisotropy of the model which complements the shape anisotropy of the 6-bead model. The critical point noticeably depends on the anisotropy, and its effect is quantified by studying the deviations of the reduced second virial coefficients at the critical point from the Noro-Frenkel law for isotropic systems.

CPP 2.10 Mon 12:15 H 0107

Single Atom Catalysis in aqueous conditions: enhanced interfacial water dissociation on a Fe-porphyrin graphene defect — •Laura Scalfi[1], Maximilian R. Becker[1], Roland R. Netz[1], and Marie-Laure Bocquet[2] — [1]Freie Universität Berlin, Berlin, Germany — [2]Ecole Normale Superieure, Paris, France

SAC or Single-Atom-Catalysis is an expanding field of heterogeneous catalysis and is particularly relevant for electrocatalysis in aqueous solutions. In SAC, the catalytically active metallic sites are reduced to single metal ions that are typically supported on a carbon scaffold. It therefore consumes less metallic material, which is an important environmental and economic factor.

Ab initio modelling and experiments mostly propose two types of defects around single metallic sites on graphene scaffolds with pyridine-like or porphyrin-like motives. Most fundamental studies however neglect the solvating water molecules. Here, we investigate how the liquid interfacial water environment interacts with a single Fe ion using extensive spin-polarized density-functional-theory molecular dynamics simulations. We show that both the porphyrin and pyridine Fe SACs spontaneously adsorb two interfacial water molecules from the solvent on opposite sides and unveil a different catalytic reactivity of the two hydrated SAC motives: while the Fe-porphyrin defect eventually dissociates an adsorbed water molecule under a moderate external electric field, the Fe-pyridine defect does not convey water dissociation. This work highlights the major role that solvents can play and the importance of including them explicitly in molecular studies.

CPP 2.11 Mon 12:30 H 0107

Ballistic-Diffusive Heat Transport Crossover in Molecular Junctions — •Pablo M. Martinez, Oscar Mateos, Oscar Gutiérrez-Varela, Juan Carlos Cuevas, and Guilherme Vilhena — Dpto. de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain

Understanding and controlling heat transport at the nanoscale is arguably one of the largest pending challenges of Nanoscience. The field has witnessed a renewed interest with recent spectacular experiments including measuring heat transport through single-atom contacts, then through single-molecule junctions. However, a full understanding of the novel and exotic heat transport phenomena at these scales remains elusive, thus hindering a de-novo design of novel nano-materials.

In this work, we combined advanced all-atom non-equilibrium simulations to achieve detailed insights into heat transport in benchmark alkane single-molecule chains ranging from few atoms up to 4 μm-long chains. Our simulations quantitatively reproduce experimental data, but most importantly they provide a detailed understanding on the breakdown of Fourier's classical law as a new form of coherent heat transport emerges (ballistic). This coherent transport is found to persist even in micron-sized contacts and in the presence of major defects.

Spectral decomposition of heat flux unveils the non-local nature of this phenomenon thus paving the road for chemically engineering heat transport at the nanoscale. Alternatively, we also explore other strategies (force and mass) for controlling the transport regime (ballistic or diffusive) and overall conductance of alkane chains.

CPP 2.12 Mon 12:45 H 0107

Viscosity of flexible and semiflexible ring melts - from molecular origins to flow-induced segregation — •Ranajay Datta, Fabian Berressem, Friederike Schmid, Arash Nikoubashman, and Peter Virnau — Institute of Physics, Johannes Gutenberg University, Staudingerweg 9, 55128 Mainz, Germany

We investigate with numerical simulations the molecular origin of viscosity in melts of flexible and semiflexible oligomer rings in comparison to corresponding systems with linear chains. The strong increase of viscosity with ring stiffness is linked to the formation of entangled clusters which dissolve under shear. This, together with an orientation of rings in shear direction lead to pronounced shear-thinning and non-Newtonian behaviour. Viscosity in linear chains on the other hand is associated with entanglements between chains which also dissolve under shear. While mixtures of flexible and semi-flexible rings mix under equilibrium conditions, differences in rheological properties induce separation under flow. This phenomena has potential applications in microfluidic devices and could be used to segregate stiffer semiflexible ring polymers from their fully flexible counterparts of similar mass and chemical composition.

CPP 3: Crystallization, Nucleation and Self-Assembly I

Time: Monday 9:30–12:45 Location: H 0110

Invited Talk CPP 3.1 Mon 9:30 H 0110

Flexibility, connectivity, and topological constraints in polymer crystallization — •Toshikazu Miyoshi — The University of Akron, School of Polymer Science and Polymer Engineering, Akron, OH, United States

Since Keller's finding of single crystals in 1957, numerous research has been conducted in experimental, theoretical, and computational aspects in polymer crystallization. The accumulated experimental results have been used to develop polymer crystallization theories as well as have gradually shifts researchers' primary interest from the crystalline structure itself to the crystal-amorphous interface and amorphous structure. Connectivity, flexibility, and topological constraint are important structures to distinguish the uniqueness of long polymer chains from small organic molecules as well as large biomacromolecules, proteins. Chain-folding structure of semicrystalline polymer is one of key structures to reflect flexibility, connectivity, and topological constraint during crystallization. In this talk, the PI will present the impacts of flexibility, connectivity, and topological constraint on the chain-folding structure of semicrystalline polymers during crystallization. The molecular level structure is used to understand the crystallization mechanisms in a dilute solution as well as in a highly condensed melt.

CPP 3.2 Mon 10:00 H 0110

Crystallizability of free and tethered chains in nanometer-sized droplets — •Wing Kit Or, Alaa Hassan, and Martin Tress — Peter Debye Institute for Soft Matter Physics, Leipzig University, Leipzig, Germany

Although the crystallization of polymers has been investigated for decades, it is not yet fully understood. One way to gain more insight is to study the differences between bulk and confined polymer, focusing on how crystallization characteristics change depending on the size and type of confinement. Until now, most studies have used confinement in thin films, small droplets, or nanopores. We prepared separated aggregates as small as ten chains on average each to characterize their individualized crystallization by probing the change in orientational polarization using a nanostructured electrode arrangement. For that, a regular pattern of well separated gold nanodots was deposited on a silicon substrate to chemically graft end-functionalized polymer chains to these nanodots. In contrast to nanometer-sized spin-cast polymer droplets (prepared as reference), the grafted aggregates exhibit no signs of crystallization. This may be attributed to several constraints like restricted chain configuration, limited chain motion, too wide chain spacing, or altered interfacial energy due to the presence of the gold surface. Preliminary results suggest that spatial constraints which prevent crystalline conformations are dominating. In principle, this approach will enable to study aggregates of fewer chains down to individual ones, which until now was accessible only to computer simulations.

CPP 3.3 Mon 10:15 H 0110

Crystallization kinetics of polyamide 10.12 from Ultra-Fast Scanning Calorimetry — •Rene Sattler and Mario Beiner — Fraunhofer IMWS, Walter-Hülse-Str. 1, 06120 Halle (Saale)

This report is focusing on the influence of isothermal and non-isothermal crystallization conditions on the crystalline states of polyamide 10.12 occurring in different polymorphic states. Results from Ultra-Fast Scanning Calorimetry (UFSC) are reported. $Isothermal$ crystallization experiments at temperatures $T_{\mathrm{c,iso}}$ below the Brill transition temperature (T_{B} = 90 °C, known from previous X-Ray Diffraction studies ^{1}) show two distinct melting peaks while a single melting peak is found after isothermal crystallization at temperatures $T_{\mathrm{c,iso}} \geq T_{\mathrm{B}}$. Two-step isothermal measurements at selected temperatures provide further evidence for the formation of two distinct phases below and above T_{B}. Indications for melting of the non-stable α phase above T_{B} in UFSC heating scans are discussed. $Non-isothermal$ crystallization experiments with various combinations of cooling and heating rates show that (i) crystal growth and (ii) nucleation can be suppressed completely. The critical cooling rate $q_{\mathrm{cool,crit}}$, at which crystallization during cooling is prevented, is about 1,500 K/s. Interestingly, cold crystallization during heating can be also suppressed if $q_{\mathrm{cool}} \geq q_{\mathrm{cool,crit}}$ and a sufficiently fast heating rate is subsequently used. The results will be discussed considering thermodynamics and relevant crystal nucleation and growth rates.

(1) R. Sattler, V. Danke, M. Beiner, *Macromol. Chem. Phys.* 224, **(2023)**, 2200433.

CPP 3.4 Mon 10:30 H 0110

New in situ X-ray experiments to investigate shear-induced crystallization effects in thermoplastics — •Anna Katharina Sambale[1], Eric Euchler[1], Kai Uhlig[1], Regine Boldt[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 thermo-rheological conditions during the processing of semi-crystalline thermoplastics have a significant influence on their microstructure and, therefore, on the performance of the final product. During processing, inhomogeneous flow fields affect the polymer melt with different shear conditions, which significantly influence the crystallization behavior during cooling and solidification. Although studies have already been conducted on the crystallization behavior of polymer melts under shear, some interactions are still unknown, for example, the influence of (local) process conditions in commercial technologies, such as melt extrusion, on the crystallization behavior of polymorphic thermoplastics. To investigate such kind of interactions, a new experimental setup has been realized to investigate the structure formation of polymer melts in situ by synchrotron X-ray scattering. In this contribution, the first results are presented on the structure formation of iPP. Owing to the high temporal and spatial resolution, new insights into the shear-induced crystallization behavior of iPP under variations of the process parameters have been achieved.

CPP 3.5 Mon 10:45 H 0110

Infrared Scanning Near-Field Spectroscopic Studies of Self-Assembled Nanostructures Based on Photo-Crosslinkable Block Copolymers — •Nadine von Coelln[1], Britta Weidinger[2], Christian Huck[1], Irene Wacker[3], Ronald Curticean[3], Rasmus R. Schröder[3], Eva Blasco[2], and Petra Tegeder[1] — [1]Institute for Physical Chemistry, Heidelberg University, Germany — [2]IMSEAM, Heidelberg University, Germany — [3]BioQuant, Heidelberg University, Germany

Block copolymers, are materials known for their ability to self-assemble into a variety of morphologies on the nanometer scale. The self-assembly of block copolymers has been extensively investigated for 2D thin films, however, less attention has been paid to 3D bulk morphologies. In this work, long-range ordered 3D bulk morphologies of a well-defined diblock copolymer consisting of polystyrene and a methacrylate-based copolymer decorated with photo-crosslinkable units were prepared via solvent annealing. The internal lamellar or cylindrical nanostructures are studied based on infrared scanning near-field optical microscopy (IR-SNOM), which offers the unique possibility of infrared chemical imaging and spectroscopy with a spatial resolution down to around 20 nm. We demonstrate that by irradiation at an independently addressable absorption band of a polymer block, it is possible to chemically image the blocks' nano-ordered spatial arrangement. By changing which polymer block is excited, a switch of the relative optical phase, related to the local absorption, is observed, revealing a strong phase segregation via spectroscopic contrast.

CPP 3.6 Mon 11:00 H 0110

Strong light-matter interaction to control intermolecular interaction and correlation — Matteo Castagnola[2], Tor Haugland[2], Enrico Ronca[3], Henrik Koch[2], and •Christian Schäfer[1] — [1]Department of Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden. — [2]Department of Chemistry, Norwegian University of Science and Technology, 7491 Trondheim, Norway. — [3]Istituto per i Processi Chimico Fisici del CNR (IPCF-CNR), Via G. Moruzzi, 1, 56124, Pisa, Italy.

Chemistry is the realm of atomic and molecular interactions, acting according to rules that we often perceive as set in stone. Optical environments, in particular the strong coupling of molecules with them, are capable to modify those interactions [1,2,3] which provides means to control chemistry itself. We provide a brief overview of the fascinating experimental accomplishments that include control over crystalization, ionic conductivity, and the reaction rate. Furthermore, we discuss how strong coupling is able to alter correlation between molecules and influences solvation and aggregation structures [4].

[1] PNAS, 116 (11), 4883, (2019). [2] J. Chem. Phys. 154, 094113 (2021). [3] arXiv:2311.09739v1. [4] M. Castagnola, T. Haugland, E. Ronca, H. Koch, C. Schäfer, to be submitted (2024).

15 min. break

CPP 3.7 Mon 11:30 H 0110

X-ray scattering techniques to study the nucleation and growth of anisotropic perovskite nanoparticles and 2D-phases — •Bert Nickel, Kilian Frank, Nina Henke, and Alexander Urban — Fakultät für Physik, Ludwig-Maximilians-Universität München

Lead halide perovskites are an emerging materials class for optoelectronic applications. Due to the ionic character of this semiconductor material, nucleation and growth processes differ profoundly from covalent semiconductor materials such as Si or GaAs. Successful solution based synthesis schemes provide shape and orientation control which is difficult to rationalize. We employ in-situ x-ray studies, especially small angle x-ray scattering (SAXS) and Bragg diffraction to study such non-classical nucleation pathways. Within this approach, we identify the water air interface [1] and internal interfaces in colloidal mesophases as driving forces for nucleation and growth.

[1] Elucidating the Origins of High Preferential Crystal Orientation in Quasi-2D Perovskite Solar Cells Lehner, L. E., Demchyshyn, S., Frank, K., Minenkov, A., Kubicki, D. J., Sun, H., Hailegnaw, B., Putz, C., Mayr, F., Cobet, M., Hesser, G., Schöfberger, W., Sariciftci, N. S., Scharber, M. C., Nickel, B., Kaltenbrunner, M. Advanced Materials 35 (5) 2208061 (2023)

CPP 3.8 Mon 11:45 H 0110

Effect of Perovskite Nanocrystal Nucleation Seeds on Microstructure and Crystallization Pathways in Organic-Inorganic Halide Perovskite Thin Films — •Altantulga Buyan-Arivjikh[1], Matthias Schwartzkopf[2], Sarathlal Koyiloth Vayalil[2], Stephan V. Roth[2], Guangjiu Pan[1], Jinsheng Zhang[1], Zhuijun Xu[1], Thomas Baier[1], Yanan Li[1], and Peter Müller-Buschbaum[1,3] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]DESY, 22604 Hamburg, 22607, Germany — [3]MLZ, TUM, 85748 Garching, Germany

Organic-inorganic halide perovskites have gained a huge interest in the scientific community owing to their favorable optoelectronic properties combined with their ease of production and abundance of raw materials. In many cases, polycrystalline thin films are fabricated for which thin film crystallinity and morphology are key factors affecting the perovskite properties. In this work, we present a novel approach for improving the thin film quality by employing external perovskite nanocrystals as seeds in slot-die coated formamidinium lead iodide thin films. Grazing incidence wide angle X-ray scattering (GIWAXS) measurements show that the seed crystals improve the thin film texture by inducing a preferred crystallite orientation. Furthermore, we reveal a new crystallization pathway in seeded thin films with respect to unseeded ones via in-situ GIWAXS measurements.

CPP 3.9 Mon 12:00 H 0110

Electric-field effects on protein phase behavior — Debes Ray[1], Mahnoush Madani[2], Jan K. G. Dhont[1], •Florian Platten[1,2], and Kyongok Kang[1] — [1]FZ Jülich, IBI-4, Jülich, Germany — [2]HHU Düsseldorf, Faculty of Mathematics and Natural Sciences, Düsseldorf, Germany

We experimentally study the state diagram of protein solutions in the presence of a weak external alternating-current electric field. The collective behavior of the protein solutions and their response to the electric field are followed in-situ by polarized optical microscopy. The crystallization boundary and the metastable liquid-liquid coexistence curve are affected by the electric field, such that the crystallization gap is widened. Both nucleation and growth of protein crystals can be modulated by the frequency and strength of the field.

CPP 3.10 Mon 12:15 H 0110

Self-assembled Peptides Structure Mediated by Solid Interfaces — •Leila Sahebmohammadi[1], Regine von Klitzing[1], Markus Mezger[2], and Pol Besenius[3] — [1]Soft Matter at Interfaces, Department of Physics, Technical University of Darmstadt, Germany — [2]Faculty of Physics, Universität Wien, Austria — [3]Department of Chemistry, Johannes Gutenberg-Universität Mainz, Germany

This study investigates the self-assembly dynamics of thermosensitive amphiphilic dendritic C3-symmetric peptides containing lysine and glutamic acid, respectively. Using Quartz Crystal Microbalance with Dissipation (QCM-D) techniques, our observations reveal temperature-dependent layer-by-layer adsorption of the oppositely charged peptides, achieving the formation of multilayers. Atomic Force Microscopy (AFM) substantiates these findings, providing visual confirmation of the confinement distribution pattern on the surface. Simultaneously, a strategic combination of supramolecular assembly and surface confinement is explored using QCM techniques.

Lysine emerges as the optimal grafting layer, exhibiting heightened adsorption on gold (Au) and silicon (Si) surfaces. Further QCM-D investigations show the same growth increment for the oppositely charged peptides at pH 6.5. Notably, exposure to extreme pH conditions (2 or 12) induces the removal of multilayers, due to low charge density of one of the peptides. This results in a better understanding of peptide self-assembly and insights for customizing surface properties through combining self-assembly and surface confinement.

CPP 3.11 Mon 12:30 H 0110

Enhancing SERS Sensitivity and Uniformity through Directional Self-Assembly of Plasmonic Nanoparticle Lattices — •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, Technische Universität Dresden, 01062 Dresden

Despite recent developments, surface-enhanced Raman spectroscopy (SERS) applications face challenges in achieving high sensitivity and uniform signals over a large area. Using the directional self-assembly of plasmonic nanoparticles in lattice structures, we show how one can increase the SERS signal 43-fold over randomly aligned gold nanoparticles without relying on the photoluminescence of Rhodamine 6G [Seçkin et al., ACS Appl. Mater. Interfaces 2023, 15(36), 43124-43134]. We have chosen the lattice constant for an off-resonant case that matches the lattice resonance and super-radiant plasmon mode along the particle chain. Supported by electromagnetic simulations, we analyze the radiative components of the plasmon modes by varying the particle size while keeping the lattice periodicity constant. We perform polarization-dependent SERS measurements and compare them with other SERS excitation wavelengths. Using the self-assembled plasmonic particle lattice [Gupta et al., Adv. Funct. Mater. 2021, 31(36) 2105054], we have developed an effective SERS substrate that provides a significantly higher signal with 73% less surface coverage. This colloidal approach enables the cost-effective and scalable fabrication of sensitive, uniform, and polarization-dependent SERS substrates.

CPP 4: Interfaces and Thin Films

Time: Monday 9:30–12:45 Location: H 0111

CPP 4.1 Mon 9:30 H 0111

Structure and dynamics in functional polymer hydrogel films — •Lucas Kreuzer[1], Calvin Brett[2], Jacques Ollivier[3], Stephan Roth[2], André Laschewsky[4], Christine M. Papadakis[5], and Peter Müller-Buschbaum[5] — [1]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) — [2]Deutsches Elektronen Synchrotron (DESY) — [3]Institut Laue-Langevin (ILL) — [4]Universität Potsdam, Institut für Chemie — [5]TUM School of Natural Sciences, Technische Universität München

Hydrogel films made from responsive polymers are able to switch between a swollen and a contracted film state in response to slight changes in their surroundings. This behavior can be used to generate highly functional hydrogel thin films e.g., from a multi-responsive diblock copolymer model system containing a zwitterionic poly(sulfobetaine) and a nonionic poly(N-isopropyl acrylamide) block. With neutron scattering techniques, we identified discrete thin-film states, regarding their thickness and film morphology, which can be precisely tuned upon changing external stimuli such as temperature or the composition of the surrounding solvent vapor. Using this knowledge, we now focus on a nanocomposite film from cellulose nanofibrils (CNF) and the electrically conductive polymer poly(3,4-ethylenedioxythiophene):poly styrene sulfonate (PEDOT:PSS). Upon cyclic swelling and drying processes, we investigated the film morphology and internal dynamics. Moreover, the influence of temperature was studied. A first analysis already indicates a correlation between the structural properties, dynamics of water inside the film, and electrical conductivity.

CPP 4.2 Mon 9:45 H 0111

Interfacial Jetting of Microgel Dispersions Induced by Surface Acoustic Wave — •Atieh Razavi[1], Regine von Klitzing[1], Amin Rahimzadeh[1], Mehrzad Roudini[2], and Andreas Winkler[2] — [1]TU Darmstadt, Hochschulstraße 8, 64289 Darmstadt, Germany — [2]SAWLab Saxony, Leibniz Institute for Solid State and Materials Research, Dresden

This study investigates Surface Acoustic Wave (SAW)-induced jetting, focusing on microgel dispersions in acoustofluidics. While SAWs have been used by others to create jets from pure liquids, this research explores the jetting of liquids with microgels as surface active polymer networks at interfaces. The work explores how microgel softness influences interfacial stability during rapid jetting induced by SAWs. Soft microgels demonstrate superior adaptability, preventing interface disintegration and sustaining longer jets compared to stiffer particles. Furthermore, higher dispersion concentrations lead to more stable jets. At 1 wt% concentration, MG1 (microgels including 1 mol% cross-linker) creates a very long jet having normalized jet length $L/R = 8.47 \pm 0.18$, compared to pure water which has an L/R of about 6.5. These findings provide critical insights into the role of microgel softness in stabilizing interfaces during millisecond-order extensions. They highlight the potential for soft microgels to significantly impact dynamic interfacial engineering in high-speed phenomena, particularly in acoustofluidics. Understanding this interplay between microgel properties and interfacial stability holds promise for advancements in rapid droplet manipulation and diverse technological applications reliant on dynamic interface control.

CPP 4.3 Mon 10:00 H 0111

Are refractive index and relative permittivity of an interphase connected to the interfacial adhesion? — •Dorothee Silbernagl[1] and Heinz Sturm[1,2] — [1]BAM, Berlin, Germany — [2]TU Berlin, IWF, Germany

Polymer interphases usually form between bulk polymer and more rigid materials. These interphases have distinct physical properties, which can differ significantly from the polymer's bulk properties. Since the dimension of those interphases are usually in the nanometer-scale we chose atomic force microscopy (AFM) force distance curves (FDC) as technique. As sample geometry we chose thin films of poly-n-butylmethacrylate (PnBMA) with different film thicknesses between 30 and 120 nm. This allows for measuring perpendicular to the film-substrate surface with a defined distance to the interface. Additionally, substrates (Si wafers) were etched locally to change the surface' polarity (Si-O versus Si-H-temination), thus tuning the interfacial adhesion of film and substrate from weak to strong. Measuring Young's moduli of such samples we were able to show the influence of interfacial adhesion. The stronger the interfacial adhesion, the higher the substrate's contribution to the overall mechanical properties. Analysis of FDCs' attractive regime revealed that also the measured Hamaker constant correlates with interfacial adhesion, showing higher contribution from the substrate with stronger adhesion. Since the Hamaker constant is derived from refractive index n and relative permittivity ϵ we hypothesis that - depending on the polymer-substrate adhesion - the polymer interphase inherits the electrodynamic properties of the substrate.

CPP 4.4 Mon 10:15 H 0111

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 showed a deviation for both poly (bisphenol-A carbonate) (PBAC) and polysulfone (PSU), two bulky polymers containing a functional group (phenyl ring) in the backbone, compared to conventional polymers previously studied like poly-2-vinyl pyridine (P2VP). This deviation was attributed to the bulkiness of the phenyl rings. Further investigations into the influence of the adsorbed layer on glassy dynamics were conducted. The molecular mobility and glass transition for thin films of PBAC and PSU were compared to bulk samples of each polymer. Broadband dielectric spectroscopy, atomic force microscopy, and ellipsometry were primarily used and additionally supported by sum frequency generation spectroscopy.

CPP 4.5 Mon 10:30 H 0111

Investigating the Ag growth on PET foil with dcMS and HiPIMS — •Yusuf Bulut[1,2], Benedikt Sochor[1], Kristian Reck[3], Suzhe Liang[2], Zhuijun Xu[2], Alexander Meinhardt[4,5], Arno Jeromin[4], Thomas F. Keller[4,5], Andreas Stierle[4,5], Thomas Strunskus[3], Franz Faupel[3], Peter Müller-Buschbaum[2,6], and Stephan V. Roth[1,7] — [1]DESY, 22607 Hamburg — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching — [3]CAU Kiel, Chair for Multicomponent Materials, Faculty of Engineering, 24143 Kiel — [4]CXNS, 22607 Hamburg — [5]UHH Hamburg, Department of Physics, 22607 Hamburg — [6]MLZ, TUM, 85748 Garching — [7]KTH, SE-100 44 Stockholm

High Power impulse magnetron sputtering (HIPIMS) is a novel industrially-relevant deposition technique enabling increased adhesion and denser film formation of thin deposited metal layers on polymers. No pre- and post-treatment is required to achieve these properties. So far, no report has discussed the nucleation and growth process during HiPIMS deposition. In this new study, polyethylenterephthalate (PET) foil is studied under various deposition conditions. Results of simultaneous in situ grazing-incidence small angle X-ray scattering (GISAXS), grazing incidence wide-angle X-ray scattering (GIWAXS) and field emission scanning electron microscopy (FESEM) are presented.

CPP 4.6 Mon 10:45 H 0111

Controllable Capillary Assembly of Magnetic Janus Particles at Fluid-Fluid Interfaces — •Qingguang Xie[1] and Jens Harting[1,2] — [1]Helmholtz-Institut Erlangen-Nürnberg for Renewable Energy (IEK-11), Forschungszentrum Jülich GmbH, Erlangen, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Nürnberg, Germany

Self-assembly of particles at fluid-fluid interfaces is a promising route to fabricate functional materials from the bottom-up. However, directing and controlling particles into highly tunable and predictable structures, while essential, is a challenge. Here, we apply a hybrid approach combining the lattice Boltzmann, and the discrete element methods to investigate the behaviour of magnetic Janus particles adsorbed at a fluid-fluid interface interacting with an external magnetic field. Depending on their tilt angle and shape (e.g. sphere, ellipsoid), the anisotropic particles deform the interface and generate capillary dipoles or hexapoles. Driven by capillary interactions, multiple particles thus arrange into reconfigurable chain-, hexagonal-lattice-, and ring-like structures, which can be actively controlled by varying the external magnetic field. We develop interface energy models to reveal the underlying mechanism and find good qualitative agreement with simulation results. Our results have implications for the fabrication of varied microstructures for use in microdevices, organic electronics, or advanced display applications.

CPP 4.7 Mon 11:00 H 0111

Elastic Capsules in Contact — •Felix Kratz and Jan Kierfeld — TU Dortmund

Contact phenomena between soft or elastic bodies are ubiquitous in nature. They are encountered in problems across the scales and include important biological processes, such as cell interactions, as well as medical applications e.g. angioplasty and drug delivery. An important hallmark in the understanding of contact mechanics is the Hertz-problem, studied and solved by Heinrich Hertz in 1881. It predicts the contact properties of bulk elastic bodies without adhesion or friction. While the contact between two bulk elastic objects is well understood by this theory, the understanding of thin-walled and pressurised elastic objects is still evolving. In this work we want to explore the contact mechanics of two thin walled, pressurised adhesive elastic capsules – with and without bending stiffness – suspended from two opposing capillaries and pressed against each other by an external force. The theoretical investigation is performed in terms of variational calculus of the appropriate free energy. We differentiate between free-slip and no-slip contact boundary conditions and derive the full set of shape and contact equations independent of the elastic constitutive law. Finally, we integrate the resulting shape equations numerically and analyse the parameter-shape-space and the force-contact-length relationship.

15 min. break

CPP 4.8 Mon 11:30 H 0111

Making stable thin nanoporous polymer films — •Hsiao-Ping Hsu and Kurt Kremer — Max-Planck-Institut für Polymerforschung, Mainz, Germany

Thin polymer films have attracted much attention due to their usefulness as supporting media in tissue engineering or as membranes in the separation processes. Thus a simulation guides processing is highly desirable. Starting from a fully equilibrated free-standing thick film of highly entangled polymer melts based on a weakly semiflexible bead-spring model [1], we apply a simple "biaxial expansion" deformation mechanism to stretch the film. For the present study the film is of thickness of several radii of gyration of the chains and the glass transition temperature T_g is the same as in the bulk case [2]. We analyze the local morphology, the void formation and its stabilization upon cooling after expansion all the way well below T_g. Motivated by these simulations a similar process is applied experimentally on films of highly entangled polystyrene and compared to simulations. Our results show an excellent qualitative and even semi-quantitative agreement [3].

[1] H.-P. Hsu, K. Kremer, J. Chem. Phys. 150, 091101 (2019); 153, 144902 (2020).

[2] H.-P. Hsu, K. Kremer, J. Chem. Phys. 159, 071104 (2023).

[3] H.-P. Hsu, M. K. Singh, Y. Cang, H. Thérien-Aubin, M. Mezger, R. Berger, I. Lieberwirth, G. Fytas and K. Kremer, Adv. Sci. 10, 2207472 (2023).

CPP 4.9 Mon 11:45 H 0111

Neutron Reflectivity of Superspreading and Non-Superspreading Trisiloxane Surfactants — •Joshua Reed[1], Séforah Carolina Marques Silva[1,2], Joachim Venzmer[2], Tatiana Gambaryan-Roisman[1], and Emanuel Schneck[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]Evonik Operations GmbH, Essen, Germany

Some trisiloxane surfactants have the remarkable property of being able to superspread: Small volumes of water rapidly wet large areas of hydrophobic surfaces. The molecular properties which govern this technologically relevant effect are still under debate. To gain a deeper understanding, the surfactant behaviour during the spreading process needs to be studied at molecular length scales. Here, we present neutron reflectivity analyses of two trisiloxane surfactants of similar structure, of which only one exhibits superspreading properties. We present an approach to determining the composition of the adsorbed surfactant layer in droplets at the solid-liquid and at the liquid-air interface, and accounting for neutron attenuation of back-reflections in thin layers. Subtle differences between superspreading and non-superspreading surfactants in the volume fractions of the self-consistent analysis might be able to explain the difference in spreading behaviour.

CPP 4.10 Mon 12:00 H 0111

Spiralling Hierarchal Structures in Chiral Lipid Monolayers Mapped with SFG Microscopy — •Alexander Fellows, Ben John, Martin Wolf, and Martin Thämer — Fritz-Haber-Institut der MPG, Berlin, Germany

The importance of phospholipids cannot be overstated. Their amphiphilic nature promotes self-assembly into two-dimensional membranes in which the hydrophobic tails tightly pack and point away from the membrane interface. Beyond this well-defined out-of-plane structure, the specific in-plane molecular arrangement also has profound implications in a vast range of physiological processes. Studies of model systems have shown condensed lipid islands (rafts) to form with a wide range of sizes and morphologies. Whilst there has been some suggestion that these domains possess in-plane molecular anisotropy and mesoscopic structural chirality, the details of their in-plane molecular orientations nevertheless remain largely unknown.

Here, we employ a newly developed SFG microscope with a novel imaging system to investigate the condensed lipid domains within monolayers with mixed chirality. We find that the domains possess curved in-plane molecular directionality within a spiralling mesoscopic hierarchal packing structure. By comparing different enantiomeric mixtures, both the molecular and spiral turning directions are shown to depend on the chirality, but with a clear deviation from mirror symmetry in the formed structures. This demonstrates strong enantioselectivity in the domain growth process, with potential connections to the evolution of homochirality in all living organisms.

CPP 4.11 Mon 12:15 H 0111

Adaptive Air-Water Interfaces with Spiropyran and Arylazopyrazole Photoswitches — •Michael Hardt and Björn Braunschweig — University of Münster, Center for Soft Nanoscience, 48149 Münster, Germany

Interfaces that can be tuned in their properties by external stimuli such as light or temperature are of great interest to drive macroscopic properties of interface-controlled soft matter materials and offer the possibility to integrate adaptive functions. Using molecular switches that respond to orthogonal triggers, the properties of fluid interfaces can be preconditioned, resulting in a low level of adaptivity that extends the possibilities of soft matter interfaces beyond being purely responsive. In this contribution, we report on air-water interfaces decorated by spiropyran (SP) and arylazopyrazole (AAP) photo-responsive surfactants. The SP surfactants increase their surface activity when irradiated with UV light, which causes a ring-closure reaction. E/Z photo-isomerization of the AAP surfactants causes a substantial decrease in surface activity and, thus, desorption from the interface. At low pH, the short thermal lifetimes of the surfactant isomers offer the use of a thermal dissipative pathway as an alternative trigger to regain the initial properties. The combination of SP and AAP surfactants allows to precondition the interface with UV light and to gain adaptive interfacial properties. This is characterized by surface tensiometry and vibrational sum-frequency generation (SFG) that provide information on interfacial composition as well as on interfacial kinetics.

CPP 4.12 Mon 12:30 H 0111

From X-ray reflectometry to surfactant surface coverage with the help of MD simulations — •Kay-Robert Dormann[1], Joshua Reed[1], Matej Kanduč[2], Benno Liebchen[1], and Emanuel Schneck[1] — [1]Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany — [2]Department of Theoretical Physics, Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia

Adsorption of surfactants to fluid interfaces occurs in numerous technological and daily-life contexts. The surfactant surface coverage Γ governs important interface characteristics like tension, viscoelastic properties, or the stability of thin foam films. Direct measurements of Γ are therefore highly desirable but have remained challenging, especially for non-ionic surfactants without easily detectable (e.g., elemental) labels

[1]. Here, we utilize atomistic MD simulations of surfactant-loaded air/water interfaces with defined Γ to obtain the associated interfacial electron density profiles. From these profiles, we compute theoretical X-ray reflectivity curves, which are then compared to experimental curves recorded with a conventional laboratory instrument. An important aspect in this procedure is the apparent interfacial roughness in experiments and simulations. For two non-ionic surfactants with previously verified force-fields [2,3] we demonstrate the suitability of this combination of experiments and simulations to deduce Γ as a function of the surfactant bulk concentration. [1] Kovalchuk et al., Langmuir 39, 3537 (2023). [2] Kanduč et al., J. Chem. Theory Comput. (2023). [3] Kanduč et al., J. Colloid Interf. Sci. 586, 588 (2021).

CPP 5: Active Matter I (joint session BP/CPP/DY)

Time: Monday 9:30–12:45 Location: H 1028

CPP 5.1 Mon 9:30 H 1028

Active Colloids as Tunable Swarmalators — •Veit-Lorenz Heuthe[1,2] and Clemens Bechinger[1,2] — [1]Fachbereich Physik, Universität Konstanz — [2]Centre for the Advanced Study of Collective Behaviour, Universität Konstanz

The complexity and functional advantages in various systems from groups of organisms to robotic swarms and digital networks hinge on spatiotemporal patterns arising from the interactions of their constituents. One approach to gain understanding of how these patterns emerge are so-called swarmalators. In this conceptual framework, individual entities exhibit both oscillatory behavior and translational motion, coupled based on their relative phase and position, yielding a diverse array of complex patterns. Here, we introduce a system of active colloids that both oscillate and translate and are coupled to each other in both speed and phase through hydrodynamic interactions. Despite the physical nature of the interactions, the system retains tunability, enabling us to systematically study the behavior of swarmalators in a real system.

CPP 5.2 Mon 9:45 H 1028

Electric field driven active colloids moving in polymeric environments — •venkata manikantha sai ganesh tanuku, peter vogel, and thomas palberg — Institute of Physics, Johannes Gutenberg University

A dilute suspension of Janus particles (JPs) in a dense viscoelastic fluid, forms a natural setting to study their dynamics in surrounding doped with macromolecules such as polymers is crucial, as most of the target application media are complex in nature. In this study, we investigate the motion of AC electric field driven SiO2-Au JPs in the presence of concentrated amounts of poly (ethylene glycol) (PEG). The transport of active particles is strongly influenced by the viscous medium and shows a dynamical jamming transition as a function of activity and medium density. For low activity, the active particle gets self-trapped in a cavity of its own making. Conversely, higher activity causes JP to push through the fluid, leaving behind a porous trail. At the given concentration of the PEG studied within these experiments two intriguing outcomes emerge: firstly, a JP can be immobilized and secondly, when two JPs move in the same direction, an unusual attraction occurs, causing the trailing JP to eventually catch up with the leading one in finite time.

CPP 5.3 Mon 10:00 H 1028

Lorentz reciprocal theorem in fluids with odd viscosity — •Yuto Hosaka[1], Ramin Golestanian[1,2,3], and Andrej Vilfan[1,4] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom — [3]Institute for the Dynamics of Complex Systems, University of Göttingen, 37077 Göttingen, Germany — [4]Jozef Stefan Institute, 1000 Ljubljana, Slovenia

The Lorentz reciprocal theorem – that is used to study various transport phenomena in hydrodynamics – is violated in chiral active fluids that feature odd viscosity with broken time-reversal and parity symmetries. Here we show that the theorem can be generalized to fluids with odd viscosity by choosing an auxiliary problem with the opposite sign of the odd viscosity [1]. We demonstrate the application of the theorem to two categories of microswimmers. Swimmers with prescribed surface velocity are not affected by odd viscosity, while those with prescribed active forces are. In particular, a torque-dipole can lead to directed motion.

[1] Y. Hosaka, R. Golestanian, and A. Vilfan, Phys. Rev. Lett. 131, 178303 (2023).

CPP 5.4 Mon 10:15 H 1028

A Stochastic Bubble Model in MIPS Active systems — •Mingqi Yan[1,2,3,4], Erwin Frey[1,4], Marcus Müller[2,4], and Stefan Klumpp[3,4] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 München, Germany — [2]Institut für Theoretische Physik, Department of Physics, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [3]Institut für Dynamik komplexer Systeme, Department of Physics, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [4]Max Planck School Matter to Life, Hofgartenstraße 8, D-80539 München, Germany

Motility-Induced Phase Separation (MIPS) is a notable phenomenon in which self-propelled particles undergo phase separation solely due to their intrinsic motility. This behavior starkly contrasts with passive systems, where active systems constantly form bubbles in liquids. Here, we introduce a stochastic bubble model to elucidate the changes in bubble area within Active Brownian Particle systems. We demonstrate that the bubble-area evolution can be described by a Langevin equation. Notably, this equation characterizes a unique category of stochastic systems: while it possesses an absorbing state, it concurrently maintains a stable nonequilibrium steady state distribution of areas.

CPP 5.5 Mon 10:30 H 1028

Dynamics and phase separation of active Brownian particles on curved surfaces and in porous media — •Priyanka Iyer, Roland Winkler, Dmitry Fedosov, and Gerhard Gompper — Theoretical Physics of Living Matter (IBI-5/IAS-2), Forschungszentrum Jülich

In biophysical systems, active particles are often exposed to curved geometries and confinement. This prompts a crucial question: How does curvature influence the emergent collective behavior of active particles? We study this question by considering the effect of curvature on an ensemble of repulsive active Brownian particles (ABPs) moving on a spherical surface. Surface curvature affects the dynamics of ABPs, as it introduces a new time scale $\tau = R/v_0$, with curvature radius R and propulsion velocity v_0, in addition to the rotational diffusion time τ_r. The time scale τ is related to a stop-and-go motion caused by the recurrent alignment of the propulsion direction with the surface normal. This implies that motility-induced phase separation (MIPS) disappears for large curvature. Moreover, the phase-separation boundary at low area fraction ϕ attains a turning point for small R, allowing for the possibility of a re-entrant behavior. The findings also have implications for understanding how curvature influences ABP dynamics in porous media, as demonstrated through a paradigmatic example involving two connected pores. Surprisingly, it is found that the different curvatures of the two pores can facilitate particle flux towards regions of high particle density and induce transient MIPS states.

[1] Iyer et al. Phys. Rev. Res. **5**, 033054 (2023).

CPP 5.6 Mon 10:45 H 1028

Giant Activity-Induced Stress Plateau in Entangled Polymer Solutions — Davide Breoni[1], Christina Kurzthaler[2], Benno Liebchen[3], Hartmut Löwen[2], and •Suvendu Mandal[3] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöhnitzer Straße 38, 01187 Dresden, Germany — [3]Technische Universität Darmstadt, Karolinenplatz 5, 64289 Darmstadt, Germany

Highly entangled active polymer solutions play vital roles in various biological processes, spanning from the intricate mechanisms of cell mitosis to the regulation of genetic transcription. We study the viscoelastic properties of highly entangled, flexible, self-propelled polymers using Brownian dynamics simulations. Our results show that the active motion of the polymer increases the height of the stress plateau by orders of magnitude due to the emergence of grip forces at entanglement points. Identifying the activity-induced energy of a single polymer and the ratio of polymer length to self-propulsion velocity as relevant energy and time scales, we find the stress autocorrelation functions collapse across Peclet numbers [1]. We predict that the long-time viscosity scales with polymer length squared, in contrast to equilibrium counterparts that scale with the cube of the polymer length [1]. These insights offer prospects for designing new materials with activity-responsive mechanical properties.

[1] D. Breoni, C. Kurzthaler, B. Liebchen, H. Löwen, and S. Mandal, https://doi.org/10.48550/arXiv.2310.02929

15 min. break

CPP 5.7 Mon 11:15 H 1028

Gravitactic bioconvection drives emergent transport and mixing in harmful algal blooms — •Soumitree Mishra[1] and Anupam Sengupta[1,2] — [1]Physics of Living Matter Group, Department of Physics and Materials Science, University of Luxembourg — [2]Institute for Advanced Studies, University of Luxembourg

Bioconvection, the active self-sustaining transport phenomenon triggered by the accumulation of motile microbes, has been long studied. Yet, if and how this collective behavior, driven by competing physico-chemical cues, impacts ecological processes including Harmful Algal Blooms (HABs) remains unexplored. Here, using a bloom-forming model phytoplankton, we present a comprehensive mechanistic study on the biophysical factors governing the emergent collective patterns and capture the eco-physiological implications of bioconvective flows. Leveraging our Ocean-On-Chip platform, together with particle tracking velocimetry (PTV) and particle image velocimetry (PIV), we uncover flow fields around isolated self-organized microbial plumes, using which we extract the spatial range of active transport. Using data-backed fluid dynamic simulations, we extract the Lyapunov exponents, revealing the mixing capacity of such plumes in confined environments. Our findings significantly advance our understanding of bioconvection's functional role in ecological contexts[1], providing a novel playground where ecology meets active matter. [Reference 1] Bioconvection mediates transport and mixing dynamics within harmful algal blooms: S. Mishra & A. Sengupta (manuscript in preparation).

CPP 5.8 Mon 11:30 H 1028

Energetic cost of microswimmer navigation: the role of body shape — •Lorenzo Piro[1,2], Andrej Vilfan[1,3], Ramin Golestanian[1,4], and Benoît Mahault[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Goettingen, Germany — [2]Department of Physics and INFN, University of Rome Tor Vergata, Via della Ricerca Scientifica 1, 00133 Rome, Italy — [3]Jozef Stefan Institute, 1000 Ljubljana, Slovenia — [4]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

We study the energetic efficiency of navigating microswimmers by explicitly taking into account the geometry of their body. We show that, whereas arguments based solely on propulsion efficiency lead to the conclusion that needle-like swimmers are most energetically efficient, disk-like swimmers rotated by flow gradients naturally follow time-optimal trajectories. The coupling between body geometry and hydrodynamics thus leads to a generic trade-off between the energetic costs associated with propulsion and navigation, which is accompanied by the selection of a finite optimal aspect ratio. We derive from optimal control theory the steering policy ensuring overall minimum energy dissipation and characterize how navigation performances vary with the swimmer shape. Our results highlight the important role of the swimmer geometry in realistic navigation scenarios.

CPP 5.9 Mon 11:45 H 1028

Optimal motility strategies for self-propelled agents to explore porous media — •Christoph Lohrmann and Christian Holm — Institute for Computational Physics, University of Stuttgart, 70569 Stuttgart, Germany

Micro-robots for, e.g., biomedical applications, need to be equipped with motility strategies that enable them to navigate through complex environments. Inspired by biological microorganisms we recreate motility patterns such as run-and-reverse, run-and-tumble or run-reverse-flick applied to active rod-like particles in silico. We investigate their capability to efficiently explore disordered porous environments with various porosities and mean pore sizes ranging down to the scale of the active particle. By calculating the effective diffusivity for the different patterns, we can predict the optimal one for each porous sample geometry. We find that providing the agent with the ability to sense position for a certain time and to make a decision based on its observation yields a motility pattern outperforming the biologically inspired patterns for all investigated porous samples[1].

[1] Lohrmann, Holm: Optimal motility strategies for self-propelled agents to explore porous media, arXiv:2302.06709, 2023

CPP 5.10 Mon 12:00 H 1028

Chemotaxis of an active particle attached to a semiflexible cargo — •Shashank Ravichandur[1], Abhinav Sharma[2,1], and Jens-Uwe Sommer[1] — [1]Leibniz-Institut für Polymerforschung, Dresden, Germany — [2]Universität Augsburg, Augsburg, Germany

The chemotaxis of synthetic active particles in activity gradients, achieved by connecting them to other active/passive particles to form simple dimers, has been demonstrated in recent studies. These studies have been extended to synthetic active particles connected to each other to form polymer chains, which also exhibit chemotaxis. However, the study of these polymer chains in activity gradients has been limited to the Rouse model, wherein the particles are connected to each other via springs, and the excluded volume interactions are ignored. To obtain a more realistic description, we consider an active synthetic particle connected to a passive tail that is semiflexible. In such a system, the configuration of the passive tail affects the motion of the active particle. Using Langevin dynamics simulations, we show that these polymers also exhibit chemotaxis in activity gradients despite the coupling between the active particle and the passive tail. We also study the effects of the chain length and bending rigidity on the chemotactic behavior.

CPP 5.11 Mon 12:15 H 1028

How cell shape guides gliding motility — •Leon Lettermann[1], Falko Ziebert[1], Mirko Singer[1], Friedrich Frischknecht[2], and Ulrich S. Schwarz[2] — [1]IPT & Bioquant, Heidelberg University — [2]CIID, Heidelberg University

Cell motility comes in many different types, including swimming, crawling and gliding. The latter term denotes movement on surfaces or through tissues without appreciable changes in cell shape and is usually based on some kind of surface flow. Gliding motility is often used by cells that need to accomplish high speeds, including myxo- or flavobacteria as well as eukaryotic parasites from the phylum apicomplexa, in particular the causative agents of malaria and toxoplasmosis. We have developed an active particle theory which connects the self-organized surface dynamics to the global motility patterns of the glider. Our theory demonstrates that the resulting trajectories depend strongly on glider shape. Our analytical solutions and numerical simulations show that straight motion to get from A to B is unstable and predict the rotational and helical trajectories which are observed experimentally for gliding bacteria and apicomplexan parasites.

CPP 5.12 Mon 12:30 H 1028

Impact of non-reciprocity on the self-aggregation of an anisotropic colloidal system — •Salman Fariz Navas and Sabine H.L. Klapp — ITP, Technische Universität Berlin, Germany

Non-reciprocal interactions have been demonstrated to introduce interesting collective behaviour in many-body systems[1]. Recent studies involving non-reciprocal colloidal particle systems have shown to induce propulsion mechanisms[2] and cause enhanced diffusion of tracer particles[3]. Such effects can have an impact on aggregation mechanisms as well[2]. Here, we introduce non-reciprocal interactions to a self-aggregating colloidal system with direction dependent, field-induced interactions[4]. In stark contrast to the passive (reciprocal) case, non-reciprocity induces a propulsion mechanism when a pair of particles belonging to different species come in contact. We show that at low degrees of non-reciprocity the aggregation is accelerated. At higher degrees of non-reciprocity, the system even tends to phase separate leading to the coexistence of dilute, freely moving particles and dense clusters.

[1] M. Fruchart, R. Hanai, P. B. Littlewood, and V. Vitelli, Nature 592, 363 (2021).

[2] S. Fehlinger and B. Liebchen, Phys. Rev. Research 5, L032038 (2023).

[3] A. Benois, M. Jardat, V. Dahirel, V. Démery, J. Agudo-Canalejo,

R. Golestanian, and P. Illien, Phys. Rev. E 108, 054606 (2023).
[4] F. Kogler, O. D. Velev, C. K. Hall, and S. H. L. Klapp, Soft Matter 11, 7356 (2015).

CPP 6: Composites and Functional Polymer Hybrids I

Time: Monday 11:30–13:00 Location: H 0106

Invited Talk CPP 6.1 Mon 11:30 H 0106

Stretchable, redispersible, recyclable: reversible interfaces for electrically conductive hybrids and composites — •Tobias Kraus — INM - Leibniz-Institute for New Materials, Saarbrücken, Germany — Saarland University, Colloid and Interface Chemistry, Saarbrücken, Germany

Composites and hybrids with organic polymer and inorganic particle components are indispensable for modern products. This talk focuses on electrically conductive hybrids and composites. We study their structure and internal interfaces to make them reversibly stretchable, enable repair, and simplify their recycling. Reversible interfaces provide functional connections that can be released with a stimulus, for example when components must be separated at the end of product lifetime. I will first discuss fundamental results on the redispersion of agglomerated particles at different length scales. Particle deagglomeration in water and non-polar organic solvents is introduced. Reversibility at the nanometer scale is then discussed for the case of printed electronics. Inks based on hybrid particles with metal cores and ultrathin layers of conductive polymers were developed as sinter-free, inkjet-printable conductors. I will show that the particles can be re-dispersed and recovered to create new inks at the end of product lifetime. As an outlook, I will discuss the role of reversible interfaces in stretchable electronics. The 3D reconstruction of conductive networks using Focused Ion Beam-Scanning Electron Microscopy tomography and leads to first results on structure-property relations for piezoresistance and ageing after many cycles.

CPP 6.2 Mon 12:00 H 0106

Effects of the particle packing structure on the thermal conductivity of filled polymer composites — •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

For a wide range of applications, polymers are modified with granular fillers to improve thermal conductivity. In addition to the filler concentration and the thermal properties of the polymer and fillers, it is predominantly the microscopic packing structure that affects the composite's achievable thermal conductivity. The attainable microscopic packing structure is dependent upon particle shape, size distribution, and agglomeration behavior, resulting in more or less effective thermal networks. For a detailed analysis of these effects, we have developed a new microscale modeling approach in which the filler packings are represented in geometric detail. Experimentally determined size distribution and shape data of the filler particles are used as input and enable the modeling of arbitrary filler materials. In this talk, we describe the new calculation strategy, the findings from the studies that have been performed on the microstructure of the filled polymer composites, and an experimental validation of the new calculation method.

CPP 6.3 Mon 12:15 H 0106

Multi-scale model of the conductivity of diblock copolymer system filled with conductive fillers. — •Alexander Chervanyov — University of Münster, Münster, Germany

We investigate the electrical response of the insulating diblock copolymer system (DBC) filled with conductive fillers depending on the following factors: (i) composite temperature and morphology; (ii) affinities of fillers for copolymer blocks; (iii) interaction between fillers. By performing consistent phase-field and Monte-Carlo simulations of a filled DBC system, we demonstrate that the location of fillers in DBC essentially depends on the above three factors. The simulated distribution of fillers in DBC, in turn, proves to be directly related to the electrical response of the composite, calculated by the developed model. In particular, the order-disorder transition in DBC system is found to co-occur with the insulator-conductor transition in the filler network provided a sufficient difference between the affinities of fillers for dissimilar DBC blocks. The order-order transition between the lamella and cylindrical morphologies of DBC is found to cause a spike in the composite conductivity.

CPP 6.4 Mon 12:30 H 0106

The sensitive aspects of modelling polymer-ceramic composite solid-state electrolytes by molecular dynamics simulations — •Melania Kozdra[1], Daniel Brandell[1], Carlos Moyses Araujo[2], and Amber Mace[1] — [1]Uppsala University, Uppsala, Sweden — [2]Karlstad University, Karlstad, Sweden

One important category of electrolytes for solid-state lithium batteries are composites of ion conducting ceramic (e.g. LLZO) and polymeric (e.g. PEO) materials. In these, Li-ion transport phenomena at the solid-solid interfaces are crucial. Using molecular dynamics (MD) techniques, we here study an interface composed of LLZO and LiTFSI-doped PEO. Although the aim of combining these materials is to utilize the advantages of each phase, both increasing and decreasing ionic conductivity has been observed as compared to the homogeneous phases. The knowledge gap regarding ionic transport processes can to a large part be attributed to difficulties in studying the ceramic-polymer interface. Here, modelling can provide insights. One of the main challenges to overcome then, however, is to understand how a sufficiently robust atomistic model can be constructed in order to provide reliable results. Therefore, a series of MD simulations are here carried out with a variation of certain structural and pair potential parameters, to test how sensitive the outcome is to each variation. Considering that atomistic studies concerning an interface of these materials are scarce, the work will hopefully spark more in silico activities to enhance the perspectives on Li-ion transport phenomena in these composite materials.

CPP 6.5 Mon 12:45 H 0106

Non-Systematic Ion-Specific Effects in Aqueous Au Nanoparticle (NP) Suspensions and Polymer-NP Composites — •Philipp Ritzert, Alexandra Striegl, and Regine v. Klitzing — Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany

Nanocomposites based on inorganic gold nanoparticle (AuNP) inclusions inside an organic matrix (e.g. polymer brushes) are employed in various fields: catalysis, material engineering, and medicine. Despite numerous demonstrations of AuNPs agents for medical and environmental applications, real world environments still present challenges due to a wide variety of interfering stimuli, e.g. ionic contaminations. Therefore, characterisation of AuNPs response to environmental stimuli is key for the usage in real world applications. The most prominent stimulus in medical applications is the presence of salts. The human body and similar environments pose many salty problems that AuNPs composite materials often attack indirectly. To characterise the ion-specific response of different AuNPs in various salt solutions we systematically employ absorption spectroscopy, transmission electron microscopy, atomic force microscopy. Our model system relies on AuNPs of two sizes and two cappings. We monitor the ion-specific response of AuNPs in suspension for various sodium salts along the Hofmeister series (anion: F, Cl, Br, I, SCN) over time. The ion-specific response of the suspensions is highly dependent on the specific anion. In addition, we immobilise the AuNPs in a polymer brush and subsequently characterise the structural rearrangement in salt solutions.

CPP 7: Composites and Functional Polymer Hybrids II

Time: Monday 15:00–16:00 Location: H 0106

CPP 7.1 Mon 15:00 H 0106

Tracking the morphology evolution of functional magnetic hybrid diblock copolymer-nanoparticle thin films by in situ GISAXS — •Christopher R. Everett[1], Guangjiu Pan[1], Manuel A. Reus[1], David P. Kosbahn[1], Aidin Lak[2], Frank Hartmann[3], Martin Bitsch[3], Markus Gallei[3], Matthias Opel[4], Matthias Schwartzkopf[5], and Peter Müller-Buschbaum[1,6] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching — [2]TU Braunschweig, Institute for Electrical Measurement Science and Fundamental Electrical Engineering, 38106 Braunschweig, Germany — [3]Saarland University, LS Polymer Chemistry, 66123 Saarbrücken, Germany — [4]Walther-Meissner-Insitut, Bayerische Akademie der Wissenschaften, 85748 Garching — [5]DESY, 22607 Hamburg — [6]MLZ, TUM, 85748 Garching

Binary diblock copolymer-nanoparticle (DBC-NP) composites are well-established materials with significant research focused on controlling the localization of the nanoparticles into one particular polymer domain. Using this knowledge as a foundation, we investigate the fabrication of ternary DBC-NP-NP composites with two distinct types of NPs. Thin hybrid films composed of PS-b-PMMA, cobalt ferrite (CoFe2O4) NPs, and nickel oxide (NiO) NPs are fabricated by a slot-die coating technique. NP segregation during the drying process is investigated with grazing incidence small-angle X-ray scattering (GISAXS). The magnetic properties of the films are probed with a SQUID magnetometer and the ternary films show enhanced magnetic coercivity and remanence compared to the single-NP films.

CPP 7.2 Mon 15:15 H 0106

Probing Water Adsorption Mechanism in Hierarchical MOFs by In Situ Positron Annihilation Lifetime Spectroscopy — •Ahmed G. Attallah[1], Volodymyr Bon[2], Kartik Maity[1], Eric Hirschmann[1], Maik Butterling[1], Andreas Wagner[1], and Stefan Kaskel[2] — [1]Institute of Radiation Physics, Hemholtz-Zentrum Dresden-Rossendorf — [2]Chair of Inorganic Chemistry I, Technische Universität Dresden, Bergstrasse 66, Dresden D-01062, Germany

Metal-organic frameworks (MOFs) offer promise in atmospheric water harvesting due to their adjustable hydrophilicity, yet understanding water sorption mechanisms remains limited. Conventional scattering techniques struggle to pinpoint water molecule positions at high loads, posing a challenge. Our proposition introduces in situ positron annihilation lifetime spectroscopy (PALS) as a valuable method to probe water adsorption mechanisms in MOFs. We employed DUT-67-Zr and DUT-67-Hf as model systems with hierarchical pore structures and tunability via metal center and linker length variations, notable for high water uptake and enhanced stability. PALS effectively identifies stepwise filling of distinct pore sizes by water molecules in both MOFs. It elucidates pore-filling dynamics as it tracks water loading by observing changes in positron lifetime and intensity, offering insights into water-framework interactions and mobility. Our findings highlight PALS as a potent tool for investigating MOFs during water loading, facilitating new perspectives for optimizing these materials in water harvesting applications.

CPP 7.3 Mon 15:30 H 0106

Thickness-dependent efficiency of fully sprayed organic thin film thermoelectrics — •Benedikt Sochor[1,2], Simon Schraad[1,3], Linus Huber[4], Alexander Hexemer[2], Tim Laarmann[1,5], Sarathlal Koyiloth Vayalil[1,6], Peter Müller-Buschbaum[4,7], and Stephan V. Roth[1,8] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, 6 Cyclotron Rd, Berkeley, 94720, CA, USA — [3]University Hamburg, Department of Physics, Notkestr. 85, 22607 Hamburg, Germany — [4]TUM School of Natural Sciences, Chair for Functional Materials, James-Franck-Str. 1, 85748 Garching, Germany — [5]The Hamburg Centre for Ultrafast Imaging CUI, Luruper Chaussee 149, 22761 Hamburg, Germany — [6]UPES, Applied Science Cluster, 248007 Dehradun, India — [7]MLZ, TUM, Lichtenbergstr. 1, 85748 Garching, Germany — [8]KTH Royal Institute of Technology, Teknikringen 56-58, 100 44 Stockholm, Sweden

Flexible organic electronics are one of the most sought-after devices in the field of photovoltaics, sensors, smart wearables or energy harvesting. This study focuses on the relationship between thickness and thermoelectric efficiency of thin films based on the semiconducting polymer poly (3-hexylthiophene-2,5-diyl) (P3HT), which shows potential as thermoelectric generators in the ambient temperature regime when doped with chloroauric acid ($HAuCl_4$). Using ellipsometry and reflectivity data as well as thermoelectric characterizations, optimal film parameters for thermoelectric thin film devices were identified.

CPP 7.4 Mon 15:45 H 0106

Higher-order modes of deformation of magnetic gels and elastomers — •Lukas Fischer and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

Magnetic gels and elastomers - soft composite materials, consisting of a soft elastic matrix with enclosed magnetizable particles - mainly react to applied external magnetic fields by changing their rheological properties (magnetorheological effect) or by overall deformations (magnetostrictive effect). So far, mostly volume changes and straight elongation or contraction along the magnetic field direction have been the focus of previous studies in the latter case.

For spherical model systems of magnetic gels and elastomers, we evaluate, based on an analytical theory, the magnetostrictive deviation in shape of the surface [1]. We characterize these deformations by a mode expansion, going beyond the previously mentioned deformational modes. The relative importance of the resulting modes crucially depends on the employed arrangement of the magnetizable particles within the elastic material.

Our goal is to offer a collection of those arrangements with their corresponding deformational modes. Therefore, if a certain deformational mode is required, it is possible to choose that arrangement that best suits this need from the collection. In this way, we hope to support the path of these materials towards actual applications.

[1] L. Fischer, A. M. Menzel, arXiv preprint arXiv:2310.16833 (2023).

CPP 8: Polymer and Molecular Dynamics, Friction and Rheology

Time: Monday 15:00–16:00 Location: H 0107

CPP 8.1 Mon 15:00 H 0107

Viscoelastic response of cross-linked epoxy using non-affine lattice dynamics: Bridging the timescale gap — •Vinay Vaibhav[1], Timothy W. Sirk[2], and Alessio Zaccone[1] — [1]Department of Physics "A. Pontremoli", University of Milan, Via Celoria 16, 20133 Milan, Italy — [2]Polymers Branch, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21005, USA

There is a vast timescale disparity, at least six orders of magnitude, at which mechanics can be probed in simulations compared to experiments. The theoretical approach, known as Non-affine Lattice Dynamics (NALD), developed by solving the equation of motion for the non-affine displacement in a disordered environment [1], has been promising in predicting the mechanics of amorphous solids at lower frequencies, making it possible to access the experimental timescales. We use large-scale computer simulations to model an epoxy system comprised of diglycidyl ether of bisphenol A (DGEBA) cross-linked by poly(oxypropylene) diamine [2], and calculate the viscoelastic response using NALD at different frequencies and also via molecular dynamics simulations for the oscillatory shear. The NALD calculations of modulus at ultra-low frequencies match with experimental data, thus, opening a new paradigm in the field of polymer viscoelasticity research to bridge the timescale gap between experiments and theory.

[1] R. M. Elder, A. Zaccone, T. W. Sirk, ACS Macro Letters, 8(9), 1160 (2019) [2] T. W. Sirk, K. S. Khare, M. Karim, J. L. Lenhart, J. W. Andzelm, G. B. McKenna, R. Khare, Polymer 54(26), 7048 (2013)

CPP 8.2 Mon 15:15 H 0107

Relating Fractional Viscoelastic Models to Relaxation Time Spectra — •Robert Franz Schmidt[1], Horst Henning Winter[2], and Michael Gradzielski[1] — [1]Stranski-Laboratorium, Institut für Chemie, TU Berlin, Berlin, Germany — [2]Chemical Engineering and Polymer Science & Engineering, University of Massachusetts Amherst, Amherst, MA, USA

Soft matter materials frequently exhibit power-law viscoelastic responses due to a broad range of relaxation times. Classical viscoelastic models, based on series-parallel arrangements of springs and dashpots, predict exponential relaxation behavior and therefore have difficulty reproducing experimental data from power-law materials. Fractional viscoelastic models represent a second class of models that incorporate derivatives of fractional order in time. They naturally predict power-law behavior and provide an excellent description of experimental data. However, physical interpretation of the model parameters is challenging due to fractional units of time.

To elucidate the meaning of the fractional parameters, we analyze the dynamic moduli of poly(ethylene oxide) (PEO) solutions using both classical and fractional viscoelastic models. We find that the Fractional Maxwell Model provides excellent description of the experimental data with only four parameters. We derive an analytical expression for the relaxation time spectrum as a function of the fractional parameters. By relating the elusive fractional parameters to tangible relaxation time spectra, our work helps to combine the advantages of both classes of models.

CPP 8.3 Mon 15:30 H 0107

Polymer dynamics and transport of energy and matter studied by rheological NMR — •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V

The effect of external shear on transport properties and polymer dynamics are studied by rheological NMR in a Searle cell. Nanoemulsions as phase-change materials are used for storage of thermal energy. A hysteresis of melting of the oil phase is observed following the fraction of the liquid signal from the oil. This is accompanied by a transition from Newtonian flow to shear banding determined by low NMR imaging. With the more flexible and deformable droplets a deviation from a linear flow profile is seen. That is accompanied by a variation of the concentration distribution as detected by spatially resolved NMR spectra in the gap. The chain dynamics in entangled polymer melts and solutions is effectively monitored by the spin-spin relaxation time T2 that is most sensitive to slow motions like chain segment motion. in polymer melt with a chain length above the entanglement length the dominating effect is the loss of entanglements. This effect sets in only at deformation rates in excess of 1000 s-1. The behavior of solutions of polyelectrolytes depends on concentration and ionic strength. Entanglement effects are observed above the entanglement concentration only. They are enhanced when the polyelectrolytes become more flexible by screening the electrostatic interaction by the addition of salt.

CPP 8.4 Mon 15:45 H 0107

Chilling alcohol on the computer: isothermal compressibility and the formation of hydrogen-bond clusters in liquid propan-1-ol — •Robin Cortes-Huerto, Luis A. Baptista, Mauricio Sevilla, and Kurt Kremer — Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

Molecular dynamics simulations have been performed to compute the isothermal compressibility κ_T of liquid propan-1-ol in the temperature range 200 - 300 K. A change in behaviour, from normal (high T) to anomalous (low T), has been identified for κ_T at $210 < T < 230$ K. The average number of hydrogen bonds (H*bond) per molecule turns to saturation in the same temperature interval, suggesting the formation of a relatively rigid network. Indeed, simulation results show a strong tendency to form H*bond clusters with distinct boundaries, with the average largest size and width of the size distribution growing upon decreasing temperature, in agreement with previous theoretical and experimental studies. These results also emphasise a connection between the behaviour of and the formation of nanometric structures.

CPP 9: Crystallization, Nucleation and Self-Assembly II

Time: Monday 15:00–17:15 Location: H 2032

CPP 9.1 Mon 15:00 H 2032

Branches, Tie Chains and Entanglements in Bimodal Polyethylene Single Crystals under Uniaxial Tensile Strain — William S. Fall[1], Jörg Baschnagel[2], and •Hendrik Meyer[2] — [1]Laboratoire de Physique des Solides - UMR 8502, CNRS, Université Paris-Saclay, 91405 Orsay, France — [2]Institut Charles Sadron - UPR22, CNRS, Université de Strasbourg, France

Short chain branched, bimodal polyethylene resins are relatively resistant to failure, due to their base material strength, when compared to other unimodal or linear compounds. The relationship between molecular level architecture and the mechanical properties of bimodal, branched PE resins is however relatively poorly understood. Using coarse-grained molecular dynamics simulations and a united-monomer model of PE, single well-aligned multi-lamella PE crystals are grown [1], using self-seeding and drawn to mimic uniaxial tensile testing. During deformation, the crystallinity, tie-chain and entanglement content are continuously monitored and correlated with the stress-strain curves obtained and mechanical properties. In addition, the dependence of all metrics on the rate of deformation and direction of drawing are also investigated, such a study is only possible due to the well-aligned PE crystals utilized here [1]. The elastic modulus of well-aligned PE crystals is strongly dependent on the direction of deformation. In the equivalent multi-domain systems, grown by continuous-cooling, such trends are almost completely hidden.

[1] Fall, W. S.; Baschnagel, J.; Benzerara, O.; Lhost, O.; Meyer, H. ACS Macro Letters 2023, **12**, 808-813.

CPP 9.2 Mon 15:15 H 2032

n-Alkanes on graphite-like substrate: Flat-histogram Monte Carlo investigation of prefreezing — •Timur Shakirov — University of Halle, Halle, Germany

In this investigation, we explore the prefreezing phenomenon [1], characterized by the formation of a thermodynamically stable thin frozen layer in polymer melts on substrates, occurring at temperatures above the bulk crystallization temperature. We consider short n-alkanes [2] in contact with graphite-like substrates. Employing flat-histogram Monte Carlo simulations [3,4], we analyze the influence of the interaction strength between the polymer and the substrate with a graphite-like lattice structure. Our research estimates the prefreezing temperature's dependence on the substrate-polymer attraction strength, providing a possibility to determine the minimal interaction threshold for prefreezing and estimating its asymptotic behavior at extremely strong attraction. The flat-histogram techniques enable a model-independent estimation of the system's free energy landscape. The outcomes of this study are compared against phenomenological theory [1] of prefreezing transition.

[1] O. Dolynchuk,M. Tariq, T. Thurn-Albrecht, J. Phys. Chem. Let. 10 (2019) 1942-1946.

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

[3] F. Liang et al, J. Am. Stat. Assoc. 102 (2007) 305-320.

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

CPP 9.3 Mon 15:30 H 2032

How to distinguish crystal symmetries in coarse-grained computer simulations of polymer crystallization in melts? — •Evgeniia Filimonova, Timur Shakirov, and Viktor Ivanov — Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany

We report on our recent developments in comprehensive analysis of crystalline structures arising during crystallization in polymer melts. Using flat histogram Monte Carlo simulations of a coarse-grained model, we obtain a very large number of (partially) crystalline conformations for low energies. We faced with the problem of distinguishing between different crystalline symmetries using the traditional well-known analysis based on bond order parameters, first suggested by Steinhardt and later improved by many authors, especially due to thermal noise. Additionally, some deformations of symmetries appear to be caused by inavoidable finite size effects. We have developed a new approach to calculate the bond order parameters using improved averaging of coordinates of particles, including a new method for visualization of local crystalline ordering on small scales. As a result, we were able to observe the coexistence of domains with different local crystalline symmetries, which had not previously been reported in the literature.

CPP 9.4 Mon 15:45 H 2032

Nucleation patterns of polymer crystals analyzed by machine learning models — •Atmika Bhardwaj[1,2], Jens-Uwe Sommer[1,2], and Marco Werner[1] — [1]Institut Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden, Germany — [2]Institute für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01062 Dresden, Germany

We employ unsupervised machine learning algorithms to investigate conformation patterns during polymer crystallization from undercooled melts using simulation data obtained from coarse grained molecular dynamics simulations. Our focus is on data-driven techniques that establish decision boundaries to detect the crystalline state of individual monomers without any prior knowledge, as opposed to classical methods that position these boundaries based on the analysis of stem length distributions [C. Luo and J.-U. Sommer, *Macromolecules* **44** (2011), 1523]. We utilize self-supervised auto-encoders to compress local conformation fingerprints of individual monomers. We show that the compressed fingerprints are organized in a lateral map that can be associated with the degrees of conformation and orientation order in the monomer's environment. The Gaussian mixture model allows to distinguish the crystalline from the amorphous phase by identifying a dense region within that map that reflects the reduced degrees of freedom. The high specificity of the method allows us to uncover the intricate temporal patterns related to crystalline order, even before any clear indications of the transition became evident in thermodynamic properties, such as specific volume.

15 min. break

CPP 9.5 Mon 16:15 H 2032

Influence of Cross-Linking and Deformation on Polymer Crystallization and Melting — Huzaifa Shabbir[1], Michael Lang[1], •Marco Werner[1], and Jens-Uwe Sommer[1,2] — [1]Institut Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Institute für Theoretische Physik, Technische Universität Dresden, Germany

We investigate the influence of the degree of cross-linking and deformation on polymer crystallization and melting behavior by means of molecular dynamics simulations. The crystallization and melting are carried out in constant strain conditions. Different properties such as specific volume, crystallinity, orientation order, and stress are studied as a function of temperature. These properties serve as key indicators, offering insights into both the microscopic and macroscopic behavior of the polymer system during the processes of crystallization and melting. Our simulation data confirms that deformation in the melt induces a pre-alignment of polymer chains in the direction of deformation, acting as a driving force for early crystallization in the deformed system. Additionally, we observe that higher degrees of deformation lead to an increase in stem length within the system, consequently higher temperatures are required for complete melting. The crystallinity exhibits an increasing and decreasing behavior in response to higher degrees of deformation and cross-linking, respectively. These findings have implications for tailoring material properties through controlled deformation and cross-linking, offering opportunities for the design of polymers with programmed mechanical response.

CPP 9.6 Mon 16:30 H 2032

Characterisation of the different polymorphs of syndiotactic polystyrene using data-driven methods — •Atreyee Banerjee[1], Tristan Bereau[2], and Joseph F. Rudzinski[1,3] — [1]Max Planck Institute for Polymer Research, Mainz, Germnay — [2]Heidelberg University, Germany — [3]Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin

Syndiotatic polysterene (sPS) exhibits complex polymorphic behaviour, resulting in rugged free energy landscapes (FELs). Enhanced sampling methods have the potential to remedy to explore the rugged FEL with prior knowledge of collective variables (CVs) that can resolve the relevant transition pathways, typically identified through extensive physical or chemical expertise. Recently, data-driven methods have attracted considerable attention for learning relevant CVs without significant a priori insight. In this work, we adapt an atomic representation used in machine learning to efficiently describe the local environment of sPS monomers. These descriptors do not require the incorporation of excessive system-specific intuition and demonstrate good transferability properties. We then investigate low-dimensional projections from methods of varying complexity: Principal Component Analysis (linear projection), Uniform Manifold Approximation, and Projection (manifold learning). These dimensionality techniques, in conjunction with clustering, provide physically meaningful polymorphic states.

CPP 9.7 Mon 16:45 H 2032

Investigating the Crystallization Behavior of Polymer Nanocomposites Through Molecular Dynamics Simulations — •Hailong Yu[1,2] and Jens-Uwe Sommer[1] — [1]Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, 01069 Dresden, Germany — [2]State Key Laboratory for Modification of Chemical Fibers and Polymer Materials, College of Materials Science and Engineering, Donghua University, 201620, Shanghai, China

Using molecular dynamics with the CG-PVA model [C. Luo and J.-U. Sommer, Computer Physics Communications 2009, 180, (8), 1382-1391] and primitive path analysis, we explored the crystallization of polymer nanocomposites with varied nanoparticle concentrations. Three systems, all employing repulsive potentials but differing in the number of nanoparticles, were examined within a matrix of long polymer chains. During crystallization, it was observed that nanoparticles migrated into interlamellar regions, aligning with the amorphous phase, as evidenced by the radial distribution function (RDF) analysis. This suggests not only the spatial confinement of nanoparticles but also their displacement from PVA's crystalline domains. These results are in agreement with recent experimental observations [K. Bornani et al., ACS Macro Letters 2022, 11, (6), 818-824]. The pure system, devoid of nanoparticles, exhibited higher crystallization temperatures and crystal ratios than nanocomposite counterparts, with consistently lower entanglement lengths during both crystallization and melting. These results show nanoparticles' crucial impact on polymer crystallization, affecting thermal behavior and structure.

CPP 9.8 Mon 17:00 H 2032

Atomic imaging of the critical nucleus size of multilayer hexagonal ice growth — •Dong Guan, Tiancheng Liang, Zixiang Yan, Li-Mei Xu, En-Ge Wang, and Ying Jiang — International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China

Multilayer water ice growth is widespread and plays a significant role in various natural phenomena. An essential aspect of water ice growth is the elusive nature of the critical ice nucleus, attributed to its transient and delicate characteristics. We present the precise atomic size of the critical ice nucleus in hexagonal water ice (ice Ih) through the utilization of qPlus-based cryogenic noncontact atomic force microscopy (NC-AFM) equipped with a CO-terminated tip. Freezing samples during the growth process allows us to capture the intermediate structures involved in the growth of Ih ice. Our investigation reveals that pentamers and hexamers are the most prevalent intermediate structures, and their combination gives rise to the 3-5 cluster, which we define as the critical ice nucleus. Combined with density functional theory, we might show that the structure alteration of the 3-5 cluster results in the formation of a new core for Ih ice. This new core can expand by incorporating additional water molecules along its periphery. This research is the first achievement in elucidating the exact atomic structure of a critical ice nucleus in water. It provides valuable insights into the water freezing process and holds the potential for application to other nucleation processes.

CPP 10: Electrical, Dielectrical and Optical Properties of Thin Films

Time: Monday 15:00–16:00 Location: H 0111

CPP 10.1 Mon 15:00 H 0111

Highly Electrically Conductive PEDOT:PSS films via Layer-by-Layer Electrostatic Self-Assembly — •Muhammad Khurram, Sven Neuber, Annekatrin Sill, and Christiane A. Helm — Institute of Physics, University of Greifswald, Felix-Hausdorff-Str. 6, 17489 Greifswald, Germany

The surface coating of an implant should be an adequate bio-interface and promote cell adhesion and proliferation. To support health, the implant should be able to transport electrical impulses. The Layer-by-Layer (LbL) method - the sequential adsorption of oppositely charged macromolecules or nanoparticles - has proven effective in coating a surface. Polyelectrolytes are poor at conducting charges; therefore, electrically conductive nanoparticles are required. PEDOT:PSS nanoparticles are used. LbL films are built from polyanion PEDOT:PSS and polycation poly-diallyldimethylammonium (PDADMA) by dip coating and a flow cell. The film prepared with flow cell exhibits lower roughness, and constant electrical conductivity (230 kS/m), regardless of the number of PEDOT:PSS bilayers deposited. Films prepared with dip-coating have lower conductivity (26 kS/m), and greater roughness. However, the electrical conductivity is constant (230 kS/m) and independent of the number of deposited PEDOT:PSS/ PDADMA bilayers. The coating exhibits ohmic behavior. By clever choice of the coating method and the number of bilayers, the sheet resistance can be tuned by two orders of magnitude.

CPP 10.2 Mon 15:15 H 0111

Optimizing the thermoelectric properties of conjugated polymer thin films by dip coating induced alignment — •Andrey Butkevich, Morteza Shokrani, Imanuel Gross, and Martijn Kemerink — Im Neuenheimer Feld 225, 69120 Heidelberg

Organic semiconductors are of great current interest for thermoelectric applications due to their inherently low thermal conductivity and good Seebeck coefficient. However, reaching competitive figures of merit has proven difficult due to the common trade-off between conductivity and Seebeck coefficient. Here, we used dip coating to align the molecules during the deposition from solution and analyzed the effect of deposition parameters on the thermoelectric performance. We used P3HT thin films which were sequentially doped with F4TCNQ as model system. Dip coated films were characterized for different doping concentrations and dip coating velocities. Clearly separated evaporation and Landau-Levich regimes were established via film thickness measurements. Morphologies with aligned polymers were formed, as confirmed by X-ray diffraction and optical spectroscopy. A beneficial effect of alignment was measured both in conductivity and Seebeck effect, leading to a clear increase in the power factor compared to non-aligned spin coated films.

CPP 10.3 Mon 15:30 H 0111

In-situ GISAXS study on the correlation of strain and photoluminescence in PbS quantum dot superlattice films on flexible substrates — •Julian E. Heger[1], Wei Chen[1,2], Huaying Zhong[1], Tianxiao Xiao[1], Constantin Harder[1,3], Fabian A. C. Apfelbeck[1], Alexander F. Weinzierl[1], Regine Boldt[4], Lucas Schraa[4], Eric Euchler[4], Anna K. Sambale[4], Konrad Schneider[4], Matthias Schwartzkopf[3], Stephan V. Roth[3,5], and Peter Müller-Buschbaum[1,6] — [1]TUM School for Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]SZTU, Shenzhen, China — [3]DESY, Hamburg, Germany — [4]IPF, Dresden, Germany — [5]KTH, Stockholm, Sweden — [6]MLZ, TUM, Garching, Germany

PbS quantum dots (QDs) show high potential as active materials in diverse optoelectronic devices, such as solar cells and photodetectors. When organized into thin films, ligand-capped PbS QDs form a superlattice structure, greatly impacting their optoelectronic properties, since the interaction among adjacent PbS QDs relies significantly on their proximity. This study examines how the superlattice arrangement of PbS QDs alters when subjected to external strain. To conduct this exploration, PbS QD thin films are fabricated on flexible PDMS substrates. In-situ grazing-incidence small-angle X-ray scattering (GISAXS) alongside photoluminescence (PL) examines how these samples deform under different levels of strain. The primary objective of this study is to correlate the structural modifications induced by strain and the consequent alterations in optoelectronic performance.

CPP 10.4 Mon 15:45 H 0111

Emission characteristics of thermally evaporated Zinc Phthalocyanine molecules in a Tetratetracontane matrix — •Gunilla W. Harm[1], Uta Schlickum[2], and Tobias Voss[1] — [1]Institute of Semiconductor Technology, Technische Universität Braunschweig, Braunschweig, Germany — [2]Institute of Applied Physics, Technische Universität Braunschweig, Braunschweig, Germany

Due to their chemical and thermal stability, Phthalocyanine molecules are promising candidates for the use as molecular quantum emitters. To investigate their potential for optoelectronic devices, we studied the emission characteristics of thermally evaporated Zinc Phthalocyanine (ZnPc) molecules on semiconductor surfaces, such as GaN. When in a crystalline phase, intermolecular coupling can influence their optical properties. To reduce this effect, the molecules are diluted by embedding them into a matrix formed by the alkane Tetratetracontane (TTC). Our results indicate that the thickness of the ZnPc film, ranging from multilayers to sub-monolayers, affects the excitonic coupling between the ZnPc molecules. The absorption band between 690 nm to 800 nm shows a reduced intensity with decreasing thickness. In addition to the typical emission in the NIR range, we see another emission band around 675 nm, which is similar to that of molecules in solution. This allows us to control the intensity ratio between the two emission bands by changing the film thickness of the ZnPc in TTC.

CPP 11: Active Fluids and Microswimmers (joint session DY/BP/CPP)

Time: Monday 15:00–18:30 Location: BH-N 243

Invited Talk CPP 11.1 Mon 15:00 BH-N 243

Control of active turbulence — •Holger Stark — Technische Universität Berlin, Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Active turbulence is one of the prominent features of active matter and occurs in diverse systems such as bacterial suspensions, biopolymeric assemblies, and tissues. One of the current challenges is to control these turbulent flow patterns for powering processes at small scales.

In the first part of the talk we rely on a continuum description of active paranematics, the Doi-Edwards theory supplemented by an active stress tensor [1]. We characterize the occuring turbulent flow for extensile active stresses. Then, motivated by the possibility to control the activity of bacteria by light, we consider a square lattice of spots, where activity drops to zero. Depending on the lattice constant and the size of the spots, we identify a trapped-vortex and, most interestingly, a multi-lane flow state. The latter consists of lanes with opposite flow directions separated by a street of vortices. It displays multistability and can also appear transiently.

Second, we perform hydrodynamic simulations of a collection of active or squirmer rods moving in their fluid environment [2]. We classify their dynamic states for the pusher/puller type as a function of density and aspect ratio of the rods and observe clustering and swarming. In particular, pusher rods show active turbulence as a compromise of disordering hydrodynamic and aligning steric interactions.

[1] A. Partovifard and H. Stark, submitted.

[2] A.W. Zantop and H. Stark, Soft Matter **18**, 6179 (2022).

CPP 11.2 Mon 15:30 BH-N 243

Entropy production in active turbulence — •Byjesh N. Radhakrishnan, Thomas L. 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 relation between the magnitude of entropy production and $+1/2$ topological defects in the system. Also, we study how EPR and the properties of defects such as mean square displacement and defect lifetime vary with the activity parameter.

CPP 11.3 Mon 15:45 BH-N 243

Active turbulent mixing — •Till Welker[1], Malcolm Hillebrand[2], Ricard Alert[2], and Holger Stark[1] — [1]Institute of Theoretical Physics, TU Berlin, Germany — [2]MPI for the Physics of Complex Systems, Dresden, Germany

Mixing on the mesoscale is crucial for both microfluidic devices and living cells. Experiments backed by simulations show a significant increase in mixing efficiency caused by active turbulence.

Our goal is to enhance the theoretical understanding of active turbulent mixing by transferring theories and concepts originally developed for inertial turbulent mixing. We therefore study a defect-free active nematic model known to show universal scaling of the energy spectrum with a passive chemical diffusing and advecting in the flow.

The efficiency of mixing χ rises with both activity of the nematic A and diffusion coefficient of the chemical D. Intriguingly, as D approaches zero, mixing efficiency converges to a non-zero value $\chi_0(A)$ because smaller D are compensated by larger concentration gradients. This presents an attractive mechanism to mix poorly diffusive substances, and is also observed in inertial turbulent mixing.

The scaling of the concentration spectrum $E_c(q)$ is of great interest and has been extensively studied in the context of inertial turbulence. We demonstrate that Batchelor-Howells-Townsend theory and Batchelor theory for strongly and poorly diffusive substances can be transferred to active turbulence. As a consequence of the universal energy scaling of our active nematic, we predict universal scaling regimes for $E_c(q)$ which we validate in simulations.

CPP 11.4 Mon 16:00 BH-N 243

Simultaneous emergence of active turbulence and odd viscosity in a colloidal chiral active system — •Joscha Mecke[1,2], Yongxiang Gao[1], Gerhard Gompper[2], and Marisol Ripoll[2] — [1]Institute for Advanced Study, Shenzhen University, China — [2]Institute of Biological Information Processing and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

Active fluids display collective phenomena such as active turbulence or odd viscosity, which refer to spontaneous complex and transverse flow. We report the simultaneous emergence of these seemingly separate phenomena in experiment for a chiral active fluid composed of a carpet of standing and spinning colloidal rods, and in simulations for synchronously rotating hard discs in a hydrodynamic explicit solvent (see also Commun. Phys. 6, 324 (2023), https://doi.org/10.1038/s42005-023-01442-3). Stresses among the colloids encompass rotational and odd shear contributions absent in usual fluids. Rotational viscosity couples the colloids' rotation to translation, causing active turbulence. Odd viscosity involves a perpendicular coupling of shear stresses, leading to an effective pressure pointing into or out of the emergent vortices. We quantify the two phenomena in experiments and simulation using the same setup. Both rotational and odd viscosity originate from the same source and the system behaviour hinges on the propagation of odd stresses via long-ranged hydrodynamics. Our findings are relevant for the understanding of biological systems and for the design of microrobots with collective self-organised behaviour.

CPP 11.5 Mon 16:15 BH-N 243

Hydrodynamic synchronization of elastic cilia: How flow confinement and boundary conditions determine the characteristics of metachronal waves — Albert von Kenne, •Markus Bär, and Thomas Niedermayer — Physikalisch-Technische Bundesanstalt, Berlin, Germany

We model hydrodynamically interacting cilia by a coupled phase oscillator description by reducing the dynamics of hydrodynamically interacting elastic cilia to the slow time scale of synchronization [1]. In this framework, we determine analytical metachronal wave solutions as well as their stability and perform simulations in a periodic chain setting. The flow confinement at the wall stabilizes metachronal waves with long wavelengths propagating in the direction of the power stroke and, moreover, metachronal waves with short wave lengths propagating perpendicularly to the power stroke. In open chains of phase oscillators, the dynamics of metachronal waves is fundamentally different. Here, the elasticity of the model cilia controls the wave direction and selects a particular wave number: At large elasticity, waves traveling in the direction of the power stroke are stable, whereas at smaller elasticity waves in the opposite direction are stable. In addition, coexistence of waves traveling in opposite directions and irregular, chaotic dynamics are observed. [1] A. von Kenne, M. Bär and T. Niedermayer. Preprint, https://www.biorxiv.org/content/10.1101/2023.10.20.563276v1.full.pdf.

CPP 11.6 Mon 16:30 BH-N 243

Pattern formation in non-Newtonian active suspensions — •Henning Reinken and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Controlling spatiotemporal patterns in active matter is of essential importance in view of prospective applications. In contrast to previous studies utilizing external control such as geometrical constraints [1], we here explore the possibility of controlling suspensions of microswimmers via the internal rheological properties of the suspension. Recent work has focused on the impact of viscoelastic and non-Newtonian behavior on the dynamics of single swimmers [3], but only a limited number of studies explores the consequences for collective motion and emergent patterns. Here, employing a recent continuum model for mesoscale turbulence in microswimmer suspensions [4], we investigate the impact of non-Newtonian behavior on the pattern formation. In particular, we focus on the stabilization of regular vortex structures in otherwise turbulent suspensions without the need for external intervention.

[1] H. Reinken, D. Nishiguchi, S. Heidenreich, A. Sokolov, M. Bär, S. H. L. Klapp, and I. S. Aranson, Commun. Phys. **3**, 76 (2020)

[3] G. Li, E. Lauga, and A. M. Ardekani, J. Non-Newton. Fluid Mech. **297**, 104655 (2021)

[4] J. Słomka and J. Dunkel, Eur. Phys. J. ST **224**, 1349 (2015), Phys. Rev. Fluids **2**, 043102 (2017), Proc. Natl. Acad. Sci. U.S.A. **114**, 2119 (2017)

15 min. break

CPP 11.7 Mon 17:00 BH-N 243

Bacterial swimming strategies in a shear flow — •Valeriia Muraveva, Agniva Datta, and Carsten Beta — Potsdam University, Potsdam, Germany

By changing the configuration of their flagella, bacterial swimmers can control their direction and speed of locomotion. The soil bacterium Pseudomonas putida pushes itself forward by counterclockwise (CCW) rotation of its flagellar bundle, while clockwise (CW) rotation pulls the cell body in the opposite direction. Additionally, P. putida can wrap its bundle of flagella around the cell body to move in a screw thread fashion. However, the benefits of having different modes of swimming still remain unclear. Here, we used microfluidics in combination with fluorescence microscopy to show how the swimming behavior changes under laminar shear flow conditions. Compared to a fluid at rest, we found that in flow, swimmers prefer the pull configuration over the wrapped one (both emerging under CW flagellar rotation). Moreover, we investigated flow-induced alignment effects and compared the distributions of swimming modes and velocities in the bulk fluid and close to the fluid-substrate interface. Our results provide first insights into how bacteria adapt their swimming strategy under different flow conditions at the single-cell level.

CPP 11.8 Mon 17:15 BH-N 243

Artificial Microswimmers in locally-tuneable hydrodynamic flow fields — •Lisa Rohde and Frank Cichos — Molecular Nanophotonics Group, Peter-Debye-Institute for Soft Matter Physics, University Leipzig, Leipzig, Germany

Biological components on the microscale, which constantly consume energy can organize themselves into functional structures through interaction with their environment. Interaction potentials, temperature or composition gradients as well as flow fields play an important role in this structure formation. We would like to transfer such self-organization principles to synthetic active particles, which are a model system to mimic the function of motors in biology, but yet have only limited functionality. Here, we expose thermo-phoretic Janus particles to an environment with tuneable hydrodynamic flow fields generated by local temperature gradients. A heated paramagnetic silica particle acts as a heat source and generates a thermo-osmotic flow field due to a temperature gradient on the substrate. By controlling the temperature of the heat source, we are able to locally change the generated hydrodynamic flow field. We study the orientational dynamics and the distance of the Janus particles relative to the heat source in dependence of temperature and laser intensities. The interplay of the local flow fields with the activity of the Janus particles results in a potential that traps the Janus particles in a configuration around the heat source. We find a polarisation of the Janus particles that align with the flow field having a stable orientation relative to the heat source.

CPP 11.9 Mon 17:30 BH-N 243

Run-and-tumble motion of ellipsoidal swimmers — •Gordei Anchutkin[1], Viktor Holubec[2], and Frank Cichos[1] — [1]Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Leipzig University, 04103 Leipzig, Germany — [2]Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University, CZ-180 00 Praha, Czech Republic

The characteristic motion of bacteria, the so-called "run-and-tumble" motion, is a hallmark of living active particles. It consists of a sequence of linear directional movements and random rotations that constantly alternate based on a biochemical feedback process. In contrast to bacteria, synthetic active particles do not exhibit run-and-tumble motion, except they are forced to do so by sophisticated optical control feedback loops.

In this study, we show that self-thermophoretic Janus ellipsoids can carry out run-and-tumble-like dynamics under strong confinement. Our Janus ellipsoids are propelled along the short axis and exhibit long periods of directed motion before reversing the propulsion direction. We show that a bimodal out-of-plane angular distribution arises at high propulsion velocities, which is mainly the result of hydrodynamic wall interactions. We evaluate hydrodynamic interactions, and gravitational and optical forces to give a quantitative model of the observed dynamics. These interactions together with the slow rotational diffusional dynamics around the short ellipsoid axis provide the basis of the run-and-tumble dynamics.

CPP 11.10 Mon 17:45 BH-N 243

Microswimming under a wedge-shaped confinement — •Alexander R. Sprenger and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany

Microswimmers, both living and artificial, frequently navigate through diverse and often confined environments. Their out-of-equilibrium nature of self-propulsion and associated fluid flows lead to complex hydrodynamic interactions with their surroundings. Understanding the impact of various confinements on the behavior of self-propelled particles is crucial for gaining insights into biological phenomena and motivating advancements in microtechnologies.

In this contribution, we study the low-Reynolds-number dynamics of microswimmers confined within a wedge-shaped free-slip boundary [1]. Such scenarios naturally occur in experiments on inhomogeneously evaporating fluid flows, which form a free-standing confinement between two converging interfaces. Additionally, wedge-shaped environments possess distinctive geometric trapping and guiding properties relevant to various microfluidic applications.

Here, we present an exact solution for the resulting flow fields for various opening angles of the wedge employing the method of images. In this manner, we investigate the hydrodynamic interactions between each swimmer and the confining interfaces. We find either attraction or repulsion towards the tip of the wedge, depending on the propulsion mechanism (pusher or puller) and the opening angle of the wedge.

[1] A. R. Sprenger, A. M. Menzel (submitted).

CPP 11.11 Mon 18:00 BH-N 243

AcoDyn: Efficient computer simulations of acoustically propelled microparticles — •Adrian Paskert and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Universität Münster, 48149 Münster, Germany

For future applications in science and engineering, active microparticles have great potential. Acoustically propelled microparticles are particularly advantageous for medical applications because they operate well within medically safe intensity ranges and are generally considered biocompatible. However, due to the complexity of the flow fields generated around these particles and the high computational cost of direct computer simulations even for simple 2D particle geometries, the theoretical understanding of the particles' propulsion and dynamics is still very limited. In this talk, we will give an overview of how these particles can be simulated efficiently to enable the numerical study of complex 3D particles. Moreover, our novel software solution `AcoDyn` will be presented, along with key results we have obtained through its application.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – 283183152

CPP 11.12 Mon 18:15 BH-N 243

Opto-fluidic dynamic patterning of microparticles — •Elena Erben[1], Weida Liao[2], Antonio Minopoli[3], Nicola Maghelli[4], Eric Lauga[2], and Moritz Kreysing[1] — [1]IBCS-BIP, KIT, Karlsruhe, Germany — [2]DAMTP, University of Cambridge, UK — [3]University of Pisa, Pisa, Itlay — [4]Fondazione Human Technopole, Milano, Italy

Techniques for the precise manipulation of microscopic objects bear great potential for application in a wide range of fields, from basic biological research to microfabrication. Our method uses rapid scanning of an infrared laser beam to optically generate thermoviscous flows [1] within a sample. Combined with closed-loop control this enables the automatic positioning of a single microparticle, with a precision of up to 24 nm [2]. Our approach can be multiplexed to manipulate up to 15 particles in a parallel and dynamic fashion. Furthermore, we have found that the positioning of multiple particles can be greatly accelerated by exploiting the complex flow patterns that result from the time-sharing of different laser scan paths. We plan to combine our approach with a full analytical model of the flows [3], which we expect will further increase the precision and speed of this manipulation method, facilitating its translation to applications in the life sciences and beyond.

[1] Weinert et al. Phys. Rev. Lett. 2008; [2] Erben et al. Opt. Express 2021; [3] Liao et al. Phys. Rev. Fluids 2023.

CPP 12: Molecular Electronics and Excited State Properties I

Time: Monday 16:15–17:30 Location: H 0106

CPP 12.1 Mon 16:15 H 0106

Charge transfer dynamics in 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 spin-allowed process in organic materials, which generates two triplet excitons from a singlet exciton [1]. Therefore, materials exhibiting SF are potential candidates to improve solar cells to achieve efficiencies beyond the Shockley-Queisser limit [2,3]. To be able to harvest electrons, an acceptor is added to the SF molecule. Specifically, we examine the complex of a diazadiborine dimer [4] as donor and tetracyanoquinodimethane as acceptor molecule. Using ab-initio multireference perturbation theory, we analyse the electronic structure, which includes charge transfer and multiexcitonic states between the donor and acceptor molecule. Moreover, we perform quantum dynamical simulations using a vibronic model Hamiltonian to investigate the charge transfer dynamics from the donor to the acceptor molecule. Furthermore, we investigate the influence of individual modes on the dynamics.

[1] M. B. Smith, J. Michl, *Chem. Rev.* **110**, 6891 (2010).

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

[3] A. J. Baldacchino et al., *Chem. Phys. Rev.* **3**, 021304 (2022).

[4] T. Zeng, *J. Phys. Chem. Lett.* **7**, 4405 (2016).

CPP 12.2 Mon 16:30 H 0106

Singlet Fission Born Quintet and Triplet States for Quantum Technologies — •Naitik Panjwani[1], Kanad Majumder[2], Woojae Kim[3], Soham Mukherjee[4], Jieun Lee[3], K.C. Krishnapriya[2], Jyotishman Dasgupta[5], Andrew Musser[4], Satish Patil[2], and Robert Bittl[1] — [1]Freie Universität Berlin, DE — [2]Indian Institute of Science, IN — [3]Yonsei University, KR — [4]Cornell University, US — [5]Tata Institute of Fundamental Research, IN

Molecular systems are promising candidates for quantum information technologies due to their reproducible nature and chemical tailorability. Photogenerated spin qubits are of interest as they form highly spin-polarised initial states e.g. in molecular systems undergoing singlet fission (SF), a process which can lead to both triplet and quintet states[1]. Furthermore, these states allow for optical detection[2] strategies to be implemented. We study a series of pentacene dimers with different linkers using electron paramagnetic resonance (EPR) spectroscopy. We investigate the role of linker geometry on relative spin state yields[3] and the influence of excitation wavelength on quintet sublevel populations[4]. Furthermore, we show how some dimers exhibit long-lived quintet states, examine the coherence properties, and investigate optical detectability in these dimers. Understanding the relationship between the spin properties and molecular structure will allow for realization of SF systems for quantum technologies.

[1] L.R. Weiss et al, Nature Phys., 2017, 13, 176 [2] G. Joshi et al, J. Chem. Phys., 2022, 157, 164702 [3] K. Majumder et al, J. Am. Chem. Soc. 2023, 145, 20883 [4] W. Kim et al, arXiv:2304.05432, 2023

CPP 12.3 Mon 16:45 H 0106

Mapping Electronic Coupling in the Excited-State during Singlet Fission with Transient Two-Dimensional Electronic Spectroscopy — •Oskar Kefer[1], Pavel V. Kolesnichenko[1], Lukas Ahrens[2], Jan Freudenberg[2], Uwe H. F. Bunz[2], and Tiago Buckup[1] — [1]PCI, Universität Heidelberg, Heidelberg — [2]OCI, Universität Heidelberg, Heidelberg

Electronic coupling of an optically bright singlet- (S_1S_0) and a dark state, known as the correlated triplet pair ($^1[T_1T_1]$), is a driving factor for singlet fission (SF). Detailed insight into the nature of the coupling is gained from theoretical considerations, due to the challenging nature of experimental confirmation. Transient two-dimensional electronic spectroscopy (transient 2DES) can directly study electronic-state correlations of singlet- and triplet excitons by utilizing an actinic-pump to launch SF beforehand.

We apply transient 2DES to spiro-linked SF-sensitizers, investigating the initial transformation of S_1S_0 to $^1[T_1T_1]$. Semi-quantum mechanical simulations allow extraction of relevant interaction parameters from measured cross-correlations of excited-states. Our findings indicate a direct SF-mechanism in the dimers, facilitated by non-adiabatic coupling between S_1S_0 and $^1[T_1T_1]$. A superposition of S_1S_0 and $^1[T_1T_1]$ is formed, which shifts towards $^1[T_1T_1]$, retaining the signatures of the coupled system even after completion. The experimental evidence reinforces the notion of the two interacting electronic states in equilibrium, a feat that was so far accessible only via computational methods.

CPP 12.4 Mon 17:00 H 0106

Ab-initio study on the effect of dipolar spin-spin interactions in singlet fission — •R. K. Kathir[1], Pedro Coto[2], and Michael Thoss[1] — [1]Institute of Physics, University of Freiburg, Germany. — [2]Materials Physics Center (CFM), Spanish National Research Council (CSIC), Spain.

Interactions between triplet pair states are known to play a key role in important chemical processes. An example is singlet fission (SF), a photo-induced multiple exciton generation mechanism in which a singlet excited state transforms into a pair of triplet excitons [1]. Electron paramagnetic resonance experiments have provided evidence that this process involves the participation of singlet and quintet coupled triplet pair states [2,3,4]. In this contribution, we employ ab-initio multi-reference perturbation theory techniques to investigate the effect of the inter-triplet relative orientation, and the strength of the zero field splitting on the SF kinetics. We perform our studies on a series of modified pentacene dimers where the pentacene-like moieties are covalently bonded to a phenylene linker in ortho, meta, and para positions, shown to undergo intra-molecular SF [5]. Our results provide insight into the spin mixing in these systems, in particular regarding the fate of the coupled triplet pair state in SF.

References:

[1] Chem. Rev., 2010, 110, 6891-6936. [2] Nat. Phys., 2017, 13, 176-181. [3] Nat. Phys., 2017, 13, 182-188. [4] Nat Commun., 2017, 8, 15171. [5] S. R. Reddy, et al., J. Phys. Chem. Lett., 2018, 9, 5979-5986.

CPP 12.5 Mon 17:15 H 0106

Exploring the Mechanisms behind Non-Aromatic Fluorescence Using the DFTB Method — Gonzalo Díaz Mirón[1], •Carlos R. Lien-Medrano[2], Debarshi Banerjee[1], Uriel N. Morzán[1], Ralph Gebauer[1], and Ali Hassanali[1] — [1]ICTP, Trieste, Italy — [2]University of Bremen, Bremen, Germany

In contrast to our standard textbook spectroscopic intuition, which attributes the fluorescence in biological systems to aromatic or conjugated groups, there are intriguing cases where non-aromatic systems exhibit inherent absorption and fluorescence in the UV-visible range. Noteworthy examples include amyloid structures, individual non-aromatic amino acids and amino acids derivatives. This study aims to comprehensively evaluate the potential of the TD-DFTB method implemented in DFTB+ [1] to investigate the photophysics underlying non-aromatic fluorescence (NAF) phenomena. The focus is on amino-acid crystals, particularly L-glutamine and its chemically transformed counterpart, L-pyro-ammonium. By comparing TD-DFTB results to previous TD-DFT studies and experimental findings [2, 3], the research successfully demonstrates TD-DFTB's accuracy in capturing non-radiative decay pathways and fluorescence origins. Furthermore, TD-DFTB is utilized to explore environmental effects using a QM/MM approach, providing insights into the experimentally observed Stoke-Shift and revealing new nuances in non-radiative decay mechanisms.

[1] Hourahine, B., et al. JCP, 152(12), 124101. (2020)
[2] Stephens, A. D., et al. PNAS, 118(21).(2021)
[3] Mirón, G. D., et al. Nature Communications, 14(1), 7325. (2023)

CPP 13: Glasses and Glass Transition (joint session CPP/DY)

Time: Monday 16:15–17:45 Location: H 0107

Invited Talk CPP 13.1 Mon 16:15 H 0107

The boson peak in the vibrational spectra of glasses — •Edan Lerner — Institute for Theoretical Physics, University of Amsterdam, Science Park 904, Amsterdam, Netherlands

A hallmark of glasses is an excess of low-frequency, nonphononic vibrations, in addition to phonons. It is associated with the intrinsically nonequilibrium and disordered nature of glasses, and is generically manifested as a THz peak — the boson peak — in the ratio of the vibrational density of state (VDoS) and Debye's VDoS of phonons. Yet, the excess vibrations and the boson peak are not fully understood. In my contribution I will provide direct numerical evidence that vibrations near the boson peak consist of hybridizations of phonons with many quasilocalized excitations; the latter have recently been shown to generically populate the low-frequency tail of the vibrational spectra of structural glasses quenched from a melt and of disordered crystals. I will next use a reanalysis of experimental data, extensive computer simulations and a mean-field model, to show that the nonphononic part of the VDoS itself features both a universal power-law tail and a peak, entirely accounted for by quasi-localized nonphononic vibrations. Our results provide a unified physical picture of the low-frequency vibrational spectra of glasses, and in particular shed basic light on the origin, nature and properties of the boson peak.

CPP 13.2 Mon 16:45 H 0107

Dynamics and Timescales of Higher Order Correlations in Supercooled Colloidal Systems — •Nele N. Striker[1], Irina Lokteva[1,2], Michael Dartsch[1,2], Francesco Dallari[1], Claudia Goy[1], Fabian Westermeier[1], Verena Markmann[1], Svenja C. Hövelmann[1], Gerhard Grübel[1,2], and Felix Lehmkühler[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

There has been extensive research into the nature of the glass transition, however its mechanisms remain mostly unclear. Recent works show that long-living locally favored structures (LFS), such as icosahedral structures forming upon supercooling, may play a key role. We show results from a combined X-ray Photon Correlation Spectroscopy (XPCS) and X-ray Cross Correlation Analysis (XCCA) experiment on colloidal hard spheres in the vicinity of the glass transition [1]. We defined a new correlation function g_c probing the timescales of higher-order correlations by tracking the time evolution of the structural higher-order correlations within the sample. We observed an increase in the ratio of the relaxation times of g_c and the standard individual particle relaxation time from about 0.4 to 0.9. The increasing values suggest that the local orders within the sample are becoming more long-lived approaching the glass transition. These results indicate that not only the presence but also the lifetime of LFS grows close to the glass transition.

[1] N. Striker et al., J. Phys. Chem. Lett., 2023, 14(20), 4719-4725

CPP 13.3 Mon 17:00 H 0107

What can MD simulations tell us about the micromechanics of deformation of glassy amorphous polymers? — •Pramod Kumar Patel[1] and Sumit Basu[2] — [1]Department of Mechanical Engineering, Indian Institute of Technology, Kanpur, India — [2]Department of Mechanical Engineering, Indian Institute of Technology, Kanpur, India

Under uniaxial compression, the stress-strain responses of glassy amorphous polymers exhibit a yield drop followed by hardening at large strains. The extent of the yield drop and the steepness of the hardening response seem connected to the polymer's molecular architecture. Moreover, these materials exhibit strain rate sensitivity, pressure-dependent yielding, and somewhat peculiar unloading behaviour. The connections between the molecular architecture of the glassy amorphous polymer and its uniaxial compressive response are not well understood.

Micromechanically motivated constitutive models proposed by various authors are often able to negotiate many of the subtle aspects of the stress-strain behaviour but need to incorporate several fitting parameters to do so. We attempt to probe the physical processes and the effect of the underlying macromolecular force fields that lead to the typical stress-strain response through well-designed molecular dynamics (MD) simulations. Moreover, using a recently developed probe for quantifying the entanglement structure of the polymer, we show that the large strain uniaxial behaviour is governed by disentanglements and entanglement slips that invariably accompany deformation.

CPP 13.4 Mon 17:15 H 0107

Sampling energy landscapes through resistance fluctuations in germanium telluride glass — •Sebastian Walfort, Jakob Ballmaier, Nils Holle, and Martin Salinga — University of Münster, Institute of Materials Physics, Wilhelm-Klemm-Str. 10, 48149 Münster

Germanium telluride (GeTe) is a fragile glass former with a large electrical property contrast between a conductive crystalline phase and highly resistive glass states. It is further possible to repeatedly amorphize and crystallize a nanoscopic, confined volume by applying short voltage pulses, which makes GeTe an interesting model system for observing glassy dynamics. For instance, physical aging following melt-quenching of GeTe glass seems to manifest in a continued evolution of the electronic properties, e.g. in a power-law-like increase of the resistivity. In this experimental study, resistance serves as the observable to probe the structural dynamics of the glass. We demonstrate that, as a consequence of reducing the nanoscopic amorphous volume, individual resistance states can be resolved in time. The fluctuations between these states are measured over a wide temperature range, six orders of magnitude in time and modeled as a (hidden) Markov process. The resulting attempt frequencies and activation energies reveal a complex free energy landscape, where transitions between states are governed by both energetic and entropic contributions to energy barriers. Beyond their relevance for electronic memory applications, these results illustrate the feasibility of the experimental approach to probe the energy landscape of a glass through a fluctuating resistance

CPP 13.5 Mon 17:30 H 0107

A self-consistent current response theory of jamming and vibrational modes in low-temperature amorphous solids — •Florian Vogel, Philipp Baumgärtel, and Matthias Fuchs — University of Konstanz, Konstanz 78464, Germany

Topologically disordered solids exhibit characterisitc anomalies like sound attenuation in the absence of thermal fluctuation and deviations from Debye*s law in the density of states. We present a novel mode-coupling approach to the understanding of athermal amorphous solids, which goes beyond the usual self-consistent Born approximation. To successfully predict the correct sound attenuation, we had to take correlated fluctuations into account. The resulting first principle theory successfully describes the jammed phase. It can also be mapped to the schematic theory [1] of the Euclidean-random-matrix model introduced by Parisi and co-workers [2] and provides a sound description of the unjammed athermal phase and our predictions for the critical dynamics agree with simulations. Most importantly, we manage to describe the unjamming transition without having to rely on negative eigenvalues of the Hessian. The softness of our systems expresses itself as a vanishing dispersion relation, which always stays non-negative. Our theory is in qualitative and semi-quantitative agreement with the numerical solutions of the ERM-model.

References

[1] F. Vogel and M. Fuchs. Phys. Rev. Lett., 130:236101, 2023.

[2] M. Mézard, G. Parisi, and A. Zee. Nuclear Physics B, 559(3):689*701, 1999.

CPP 14: 2D Materials

Time: Monday 16:15–17:45 Location: H 0111

CPP 14.1 Mon 16:15 H 0111

Molecular dynamics dimulation: exploring human odorant adsorption on functionalized 2D carbon surfaces. Workflow. — •Nina Tverdokhleb[1], Li Chen[1], Arezoo Dianat[1], Rafael Gutierrez[1], Alexander Croy[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science, Dresden University of Technology, Dresden 01062, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07737 Jena, Germany

Our group explores the sensory properties of graphene and nanotubes functionalized with mucin-based smell receptors specifically designed to detect human odorant molecules. This involves a molecular dynamics simulation using the NAMD software to analyze interactions between pools of receptors and odorants in the gaseous phase. The adsorption energy of odorants on functionalized graphene is assessed using The Adaptive Biasing Force (ABF) Method [1], revealing correlations with structural characteristics. Moreover, we ascertain the receptor recovery time through the application of the Arrhenius law, and extract temporal associations from molecular dynamic trajectories. This approach holds the promise of fostering a more profound understanding of the sensory mechanisms, contributing to the development of electronic olfaction for enhanced disease detection.

[1] Eric Darve, David Rodríguez-Gómez, and Andrew Pohorille. Adaptive biasing force method for scalar and vector free energy calculations. J. Chem. Phys., 128(14):144120, 2008.

CPP 14.2 Mon 16:30 H 0111

Radioactive Tracer Diffusion through TPT-CNMs — •Neita Khayya, André Beyer, and Armin Gölzhäuser — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

In recent years, Carbon Nanomembranes (CNMs) have emerged as an innovative class of thin 2D materials known for their exceptional combination of high selectivity and permeation properties, with a particular emphasis on p-[1,1',4',1"]-terphenyl-4-thiol (TPT)-CNM. Despite significant progress in comprehending the characteristic features of CNMs, there remains a need for further clarification of their fundamental properties, which can be addressed through complementary methods. Here, we report the permeation measurements derived from concentration-gradient-driven transport of radioactive tracer molecules, specifically [3H] H_2O, [14C] $NaHCO_3$, and [32P] H_3PO_4, through TPT-CNMs. Our investigation explores into the impact of the pH value on the diffusion process. Considering concentration polarization and outgassing effects by a mathematical model, our results align with previously obtained radioactive diffusion data for a neutral pH value of 7. Interestingly, despite the electrostatic barrier associated with TPT-CNM, our observations indicate enhanced permeation of anions in the basic range of pH. This emphasizes the nuanced behavior of TPT-CNMs under varying pH conditions, shedding light on their unique permeation characteristics.

CPP 14.3 Mon 16:45 H 0111

Theoretical Studies on the Formation of Polymeric Nitrogen-containing 2D-Networks of Tricyanobenzene Derivatives on Coinage Metal Surfaces — •Alix Kaczmarek[1,2], Jörg Sundermeyer[3], and Doreen Mollenhauer[1,2] — [1]Institute of Physical Chemistry, Justus-Liebig University Giessen, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig University Giessen, Germany — [3]Chemistry Department, Philipps-University Marburg, Germany

The field of metal surface chemistry, and on-surface reactions in particular, has attracted considerable attention in recent years. The development of fundamental strategies for on-surface synthesis through the investigation of the underlying reaction mechanisms will provide a toolbox for applications in various fields such as photonics, photo- and electrocatalysis, or solar energy conversion. E.g. 2D graphene-like nitrogen-containing 'azagraphene' networks are a promising class of systems for use in nanoscale electronic devices. Here, we present the investigation of the trimerisation mechanisms of planar 1,3,5-tricyanobenzene (TCB) and 2,4,6-tricyano-1,3,5-triazine (TCT) on (111) coinage metal surfaces copper, silver, and gold, using density functional theory with dispersion correction. Our findings may provide guidance for the experimental synthesis of nitrogen-containing graphene networks and aid in the selection of suitable precursor-surface-systems.

L. Alix Kaczmarek, Michael Gottfried, Jörg Sundermeyer, Doreen Mollenhauer. Manuscript in preparation.

CPP 14.4 Mon 17:00 H 0111

Atomistic simulation of a novel non-covalent functionalized graphene-based sensor material for body odor volatilomes detection — •Li Chen[1], Nina Tverdokhleb[1], Arezoo Dianat[1], Rafael Gutierrez[1], Alexander Croy[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science, Dresden University of Technology, Dresden 01062, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07737, Jena, Germany

Detecting the body odor volatilomes (BOVs) represents a crucial step in comprehending its implications for human social interactions and healthcare. This work explores a novel mucin-based receptor functionalized graphene-based sensor material for BOVs detection through atomistic simulations. The density functional theory (DFT) investigation involves calculating the binding features of analyte-substrate interactions, including binding energy and charge transfer. These electronic properties characterize the sensing mechanisms and yield synergistically sensor signal response in the end, which could be estimated by the work function change before and after BOVs adsorption. This research enhances the fundamental understanding of the analyte-receptor interactions and potentially facilitates the selection and optimization of the receptors in pursuit of high responsiveness and excellent discrimination capabilities.

CPP 14.5 Mon 17:15 H 0111

Defect-Healed Carbon Nanomembranes for Enhanced Salt Separation: Scalable Synthesis and Performance — •Zhen Yao[1], Pengfei Li[1,2], Kuo Chen[1,2], Yang Yang[1], André Beyer[1], Qingshan Niu[3], and Armin Gölzhäuser[1] — [1]Bielefeld University, 33615 Bielefeld, Germany — [2]China University of Petroleum (East China), Qingdao 266580, PR China — [3]Shenzhen University, Shenzhen 518060, PR China

Carbon nanomembranes (CNMs), featuring a high density of sub-nanometer channels, enable superior salt separation performance compared to conventional membranes. However, defect occurrence during synthesis and transfer processes impedes their technical realization on a macroscopic scale. Here, we introduce a practical and scalable interfacial polymerization method to effectively heal defects while preserving the sub-nanometer pores within CNMs. The defect-healed CNMs exhibit exceptional performance in forward osmosis (FO), achieving a water flux of 105 L m-2 h-1 when measured with 1M NaCl as draw solution. This water flux is ten times higher than commercially available FO membranes. Through successful implementation of the defect-healing method and support optimization, we demonstrate the scalable synthesis of fully functional, centimeter-scale CNM-based composite membranes, showing a water permeance comparable to commercial membranes and a salt rejection of ˜99.8%. Our defect-healing method presents a promising pathway to overcome limitations in CNM synthesis, unlocking their potentials for practical salt separation applications.

CPP 14.6 Mon 17:30 H 0111

Theoretical Studies of the Influence of Different XC-Functionals and Dispersion Corrections on Surface Assisted Reactions and Comparison with Theory of a Higher Level

— •Kiyan Linus Haiko Pohl[1,2], Jannis Jung[1,2], and Doreen Mollenhauer[1,2] — [1]1 Institute of Physical Chemistry, Justus-Liebig University Giessen, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig University Giessen, Germany

Experimental and theoretical studies of on-surface reactions, such as the surface assisted Ulmann-coupling, have become of increasing interest in the recent years, as they provide a promising path to e. g. 2D graphene like structures . Density functional theory (DFT) is mainly used for the theoretical studies, and a variety of different exchange-correlation (XC) functional and dispersion correction combinations are available for the calculations.

We investigated combinations of 22 XC functionals and 5 dispersion corrections for the Ullmann coupling reaction of bromobenzene on the (111) coinage metal surfaces of copper, silver, and gold. We studied the influence of these combinations on different steps of the reaction. First, the lattice parameters and the structure of the molecule were calculated and compared with experimental or benchmark values (at the CCSD(T) theoretical level). Second, the adsorption energies and the distances of the molecules and radicals from the surface were also studied and compared to each other [1].

[1] Pohl, K. L. H., Mollenhauer, D., Manuscript in preparation.

CPP 15: Poster I

Wetting on Adaptive Substrates (1-3), Gels, Polymer Networks and Elastomers (4-10), Biopolymers, Biomaterials and Bioinspired Functional Materials (11-16), Complex Fluids and Colloids, Micelles and Vesicles (17-19), Charged Soft Matter, Polyelectrolytes and Ionic Liquids (20-23), Energy Storage and Batteries (24-33), Responsive and Adaptive Polymers (34-38), Wetting, Fluidics and Liquids at Interfaces and Surfaces (39-41), Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods (42-45)

Time: Monday 18:00–20:00 Location: Poster C

CPP 15.1 Mon 18:00 Poster C

Synthesis of diblock copolymer brush layers 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, Mainz, Germany — [2]Institute of Macromolecular Chemistry CAS, Prague, Czech Republic

The Youngs model describes the wetting behavior of an ideal surface. Recently, Butt et al. presented an adaptation model, which connects adaptation processes of the surface to dynamic contact angles [1]. In order to test the adaptation model, we used a tilted plate setup, which allows measuring velocity dependent contact angles. The applicability of the adaptation model was experimentally verified by using surfaces made of statistical copolymers. In a next step, we synthesize polymer 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)) or Poly(1-hexyl methacrylate) (PEtHexMA) as hydrophobic block on top of the PHEMA block [2]. By regulating the architecture and thickness of the polymer brush we tune the wetting properties systematically. In addition, we control the adaptation time of polymer brush surfaces by changing the drop-sample temperature.

CPP 15.2 Mon 18:00 Poster C

Effect of Low-Pressure Plasma-Treated Hydrophobic Surfaces on Sliding Water Drop Charge — •Fahimeh Darvish[1], Sajjad Shumaly[1], Xiaomei Li[1], Yun Dong[1], MohammadReza Khani[2], George Floudas[1], Doris Vollmer[1], and Hans-Jürgen Butt[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany — [2]Laser and Plasma Research Institute, Shahid Beheshti University, 1983963113 Tehran, Iran

Slide electrification is the spontaneous separation of electric charges at the rear of water drops sliding over hydrophobic surfaces. This research shows how plasma-treated surfaces affect water sliding electrification. Plasma treatment reduced the contact angles and drop charging. Conversely, 64% higher drop charging was achieved using sheath treatment than to pristine sample. Based on the zeta potential, Kelvin potential, XPS measurements, we attributed the effects of plasma to two processes. First, plasma chemically changed the organic topmost layer, e.g., by oxidation and etching. Secondly, charges were deposited in the topmost layer. The surface top layer charges were less negative after sheath and more negative after bulk plasma treatment. The plasma-treated effect was neutralizable. Despite the presence of a PFOTS thin layer, we discovered that the plasma effect on the substrate governs slide electrification remotely, by using different plasma powers during glass activation prior to silanization. However, the surface roughness and contact angles remained unchanged. We demonstrated that both sheath and plasma treatment increase or decrease slide electrification to almost zero while keeping other surface properties constant.

CPP 15.3 Mon 18:00 Poster C

Partially wetted PNiPAAm brushes responses to different atmospheres — •Simon Schubotz[1,2], Petra Uhlmann[1], Andreas Fery[1,2], Jens-Uwe Sommer[1,2], and Günter K. Auernhammer[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — [2]Technische Universität Dresden, 01069 Dresden, Germany

In our study, we focused on the partial wetting of co-nonsolvent polymer brushes and the dynamics of a three-phase contact line moving over such brushes. We performed wetting experiments in different atmospheres and used an ellipsometer to measure the brush's thickness to understand the impact of the atmosphere on the brush. Our findings show that PNiPAAm brushes exhibit a memory effect when depositing drops consecutively at the same position. The subsequent drops adapt the brush and change the drop's wetting behavior. In further wetting experiments, we measured water drops in an ethanol-saturated atmosphere on PNiPAAm brushes. The measurements show that an ethanol-enriched atmosphere strongly affects the memory effect reversibly. We present strategies to counter the mixing between the atmosphere and the drop.

[1] Schubotz, S., et al., Memory effects in polymer brushes showing co-nonsolvency effects. Advances in Colloid and Interface Science, 2021. 294: p. 102442.

[2] Schubotz, S., et al., Influence of the Atmosphere on the Wettability of Polymer Brushes. Langmuir 2023, 39, 14, 4872-4880

CPP 15.4 Mon 18:00 Poster C

Simulations of Weak Polyelectrolyte Hydrogels with Divalent Counterions — •David Beyer[1], Peter Košovan[2], and Christian Holm[1] — [1]Institute for Computational Physics, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Department of Physical and Macromolecular Chemistry, Charles University, 128 00 Prague 2, Czechia

We use computer simulations to study a coarse-grained model of a weak (pH-responsive) polyelectrolyte hydrogel coupled to a reservoir of small ions, including a 2:1 salt. To model the ionization equilibrium of the weak groups and the exchange of small ions with the reservoir, we make use of the recently developed Grand-Reaction Monte-Carlo method (G-RxMC). We determine the free swelling equilibrium for different concentrations of the divalent salt and pH values of the reservoir. Our simulations show that even a small amount of divalent salt can significantly inhibit the swelling of the gels due to the preferential uptake of divalent ions into the gel, effectively suppressing the swelling for salt concentrations above 10mM. Interestingly, we observe that the gels exhibit a second swelling step at very high pH-values, which is in stark contrast to the behaviour in a monovalent salt solution. This behaviour arises due to an interplay of the ion partitioning and electrostatic interactions.

CPP 15.5 Mon 18:00 Poster C

On the swelling of polymer network strands — •Michael Lang and Reinhard Scholz — Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany

Large scale computer simulations are employed to analyze the conformations of network strands in polymer networks at preparation conditions and at swelling equilibrium. Network strands in end-linked model networks are weakly stretched and partially swollen at preparation conditions as compared to linear polymers at the same polymer volume fraction. For increasing overlap of the chains, network swelling causes a non-ideal chain size $\propto N^{\nu}$ characterized by an effective scaling exponent ν approaching 7/10 on intermediate length scales. The chain size in a network consists of a fluctuating and a time average "elastic" contribution. The elastic contribution swells essentially affinely, whereas the swelling of the fluctuating part lies between the expected swelling of the entanglement constraints and the swelling of non-cross-linked chains in a comparable semi-dilute solution. The total swelling of chain size results from the changes of both fluctuating and non-fluctuating contributions.

CPP 15.6 Mon 18:00 Poster C

Impact of Curing dynamics on the Microstructure and Properties of Epoxy Thermosets — •Sampanna Pahi[1], Christian Wick[1], and Ana-Sunčana Smith[1,2] — [1]PULS Group, Institute for Theoretical Physics, IZNF, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Group of Computational Life Sciences, Ruder Bošković Institute, 10000 Zagreb, Croatia

Epoxy resins, essential in manufacturing, require an understanding of their curing kinetics for optimal properties. This study, using epoxy systems modeled with the recently developed Block Chemistry forcefield, examines the impact of reaction kinetics on polymer chain formation. We employed a QM/MM methodology to optimize local reaction kinetics at the molecular level, enhancing curing precision. Quantum analyses and simulations showed that secondary reactions prompt early branching, while primary reactions lead to linear growth before crosslinking. Further, incorporating an isomeric mixture in the pre-polymer model resulted in denser packing, mirroring experimental densities. The study also includes loop size distribution analysis within the polymer matrix, crucial for assessing material rigidity and linking microstructural characteristics to macroscopic properties, enriching our understanding of the molecular structure-material behavior relationship in thermoset polymers.

CPP 15.7 Mon 18:00 Poster C

Probing the mechanical properties of core-shell-like PNIPAM microgels — •Manmeet Kaur Sodhi and Regine Von Klitzing — Technische Universität Darmstadt

Stimuli-responsive liquid foams have a huge impact in terms of both fundamental research and technical applications such as catalysis, food technology, waste, since they allow a foam rupture on demand triggered by external stimuli. Temperature responsive. PNIPAM microgels (radii in the range of several 100 nm) are well-known to stabilize foams, and they have a volume phase transition temperature (VPTT) of about 32°C, i.e. below this temperature water is a good solvent and the microgels are swollen. By crossing the VPTT water becomes a poor solvent and the microgels shrink, their stiffness controlled by the degree of crosslinking, and their ability to stabilize liquid foams. This study focuses on the fundamental question of how important the softness/stiffness of the microgels is to stabilize foams. To achieve this, the mechanical properties of negatively charged individual microgel particles at solid/air interface as well as solid water interface has been studied. The data is complemented with the dynamic light scattering which not only gives us the quantitative understanding of including their hydrodynamic radius and polydispersity but also allows us to understand the behaviour of these microgels at lower critical transition temperature.

CPP 15.8 Mon 18:00 Poster C

Study of core-shell nanogels via molecular computer simulations — •Alla Dobroserdova[1] and Sofia Kantorovich[2] — [1]Ekaterinburg, Russia — [2]University of Vienna, Vienna, Austria

Nanogels represent a new class of smart materials. They consist of a permanently cross-linked network of dilute polymers. We consider core-shell nanogels, where the polymers in the shell can have different lengths. Considering some magnetic core particles, we make nanogels with a magnetic core. We can also consider the magnetic particles of the shell along with the magnetic particles of the core. We study how the intensity of the magnetic dipole-dipole interaction affects the magnetic and structural properties of the nanogel.

CPP 15.9 Mon 18:00 Poster C

Influence of single particle softness on the elasticity of microgel covered interfaces — •Carina Schneider, Sebastian Stock, Joanne Zimmer, and Regine von Klitzing — Department of Physics, TU Darmstadt, Hochschulstraße 8, 64289 Darmstadt

Softness strongly influences the behavior of microgels (MG) adsorbed at liquid interfaces. Therefore, it is fundamental to understand and quantify its effect via the microscopic scale on the macroscopic layer. For this purpose, we spread homogeneous and heterogeneous polyNIPAM MGs at the air-water interface of a Langmuir trough, and determine the compression isotherms. This enables the calculation of the compression dependent elasticity. We control the stiffness of the MG particles by varying the cross-linker density. To artificially increase the stiffness of the single particles we add latex particles to the system. Simultaneously, we observe the lateral structure formation, by transferring and subsequently scanning the particle layer on a Silicon wafer using atomic force microscopy. The elasticity of the particle layer at the interface exhibits a maximum as a function of the surface pressure. Counterintuitively, the maximum value increases with decreasing stiffness of the particles.

CPP 15.10 Mon 18:00 Poster C

How Ultrasound Accelerates Microgel Adsorption Kinetics at Liquid Interfaces — •Luca Mirau[1], Sebastian Stock[1], Amin Rahimzadeh[1], Sonja Wismath[2], Matthias Rutsch[2], Mario Kupnik[2], and Regine von Klitzing[1] — [1]Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 8, 64289 Darmstadt — [2]Measurement and Sensor Technology, TU Darmstadt, Merckstraße 25, 64283 Darmstadt

Poly-N-isopropylacrylamide (PNIPAM) based microgels (MGs) are surface-active and offer great opportunities as stabilizers of emulsions and foams. Due to their thermosensitive response the MGs enable also destabilization on demand. However, emulsion formation implies energy input by stirring or ultrasonication. To understand this formation process, it is important to understand the interfacial adsorption of the MGs. A fast trigger to affect the adsorption process is given by ultrasonication. The present study shows the effect of ultrasound on the adsorption kinetics of PNIPAM MGs at the water-oil interface monitored by drop shape tensiometry. The adsorption kinetics of MGs accelerates with increasing ultrasonication intensity. The variation of different parameters, such as ultrasonic frequency, MG crosslinker density, concentration, phase composition and temperature, indicates that both acoustic streaming as well as ultrasound induced deswelling of MGs due to breakage of hydrogen bonding cause this acceleration.

CPP 15.11 Mon 18:00 Poster C

Water-based lignin colloidal particle and cellulose nanofibrils hybrid films with UV-block ability by spray deposition — •Shouzheng Chen[1,2], Constantin Harder[1,3], Iuliana Ribca[4], Yusuf Bulut[1,3], Peter Müller-Buschbaum[3,5], Mats Johansson[4], Julien Navarro[2], and Stephan Roth[1,4] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — [2]Institute of Wood Science, Universität Hamburg, 20146 Hamburg, Germany — [3]Physik-Department, Lehrstuhl für Funktionelle Materielien, Technische Universität München, James-Franck-Strasse 1, 85748 Garching, Germany — [4]KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, 10044 Stockholm, Sweden — [5]Technische Universität München, Heinz Maier-Leibnitz Zentrum (MLZ), Lichtenbergstr. 1, 85748 Garching, Germany

Cellulose nanofibrils(CNFs) have hydrophilic interfaces and establish self-entangled networks, making them natural biopolymer substrate materials. Lignin is a natural UV-shielding material due to its high content of phenolic groups. We prepared hybrid films from CNFs and water-based colloidal lignin particles(CLP) by spray deposition using layer-by-layer stacking as well as premixing. The resulting nanostructures were correlated with water imbibition, UV shielding ability and visible light transparency of the films. We found that CNF acts as a directing agent in the premixed system to dominate the uniform distribution of CLP in the thin film, which allows to optimizing the visible light transparency while maintaining the UV-shielding ability.

CPP 15.12 Mon 18:00 Poster C

Coarse-grained modeling of nucleic acid coacervates —

•Soumen De Karmakar and Thomas Speck — Institute for Theoretical Physics IV, University of Stuttgart, Heisenbergstr. 3, Stuttgart 70569, Germany

Membraneless biomolecular condensates, consisting of several components such as multivalent proteins, RNA, and DNA, are ubiquitous in cellular environments. Recent in vitro studies demonstrate the condensation of single-stranded DNA (ssDNA) [1] or RNA [2] with increasing temperature reminiscent of lower critical solution temperatures (LCST) in thermoresponsive polymers. The observed LCST suggests that entropic interaction play a significant role in addition to the conventional enthalpy dominated interactions in other biomolecular condensates. To shed more light on the possible mechanism of LCST in the single component biomolecular condensates, we employ a minimal coarse-grained model and implicitly incorporating background ions that are essential for the formation of condensates. Our numerical study exhibits phase separation in line with the experiments of ssDNA and RNA. Our results provide insight into the design of hierarchical structures composed of several components of biomolecular assemblies.

[1] Merindol et al., Nat. Nanotech. 13, 730-738 (2018). [2] Wadsworth et al., Nat. Chem. (2023), 1755-4349.

CPP 15.13 Mon 18:00 Poster C

Are alginate - pullulan sponge-like composites suitable to help heal a skin wound? — •Emma Bobu[1], Klara Magyari[2], Alexandra Dreanca[3], and Monica Baia[4] — [1]Doctoral School in Physics, BBU, Cluj, Romania — [2]Interdisciplinary Research Institute on Bio-Nano-Sciences, BBU, Cluj, Romania — [3]Faculty of Veterinary Medicine, UASVM, Cluj, Romania — [4]Faculty of Physics, BBU, Cluj, Romania

A major health issue that needs to be addressed is external bleeding, which occurs every day in people around the world, due to accidents or surgery. Normally, the body reacts immediately to stop the bleeding and heal the wound, but there are deep and uncontrolled bleedings, and the body needs external help for hemostasis. First, we need to absorb the blood and keep the wound moist. The natural polymers chosen for this purpose are calcium alginate and pullulan, because of their good swelling proprieties and biocompatibility. Therefore, the final material CAlg-Pll has a sponge-like structure that absorbs the fluid to increase the viscosity and concentration of the blood in the wound while keeping the environment moist. That stops the bleeding and prevents big losses. The samples were synthesized and characterized by XRD, FT-IR, and Raman spectroscopy. For the in vitro tests, the samples were immersed in simulated body fluid to see the bioactivity, swelling ratios, and degradability and were again investigated by XRD, FT-IR, Raman spectroscopy, and SEM. The next assay was the evaluation of coagulation rate and time. The materials are stable in biological fluid, absorb the excess fluid in the wound, and are nontoxic.

CPP 15.14 Mon 18:00 Poster C

In situ X-ray studies of temperature-controlled structures in polylactic acid — •Regine Boldt[1], Laura Meinig[1], Eric Euchler[1], Anna Katharina Sambale[1], Kai Uhlig[1], Matthias Schwartzkopf[2], and Markus Stommel[1,3] — [1]Leibniz-Institut für Polymerforschung, Dresden, Germany — [2]Deutsches Elektronen Synchrotron DESY, Hamburg Germany — [3]TUD Dresden University of Technology, Dresden, Germany

Polylactic acid (PLA) is a frequently used biopolymer. It is used, for example, as films for food packaging and in agriculture in the form of mulch films. PLA is also used in medicine as implant or suture material. To precisely control application-specific material properties, a better understanding of the formation of relevant structures and identifying influential process parameters is essential. In this work, we focused on investigating the formation of crystalline structures at different temperatures. It is known that PLA crystallizes in two different modifications depending on the temperature: (i) the metastable α'-phase and (ii) the thermodynamically stable α-phase. We investigated the formation of the different phases using in situ synchrotron X-ray scattering experiments. Using a newly developed experimental setup, PLA was heated to melt and then cooled to different temperatures and monitored the crystallite formation as a function of time. As a result, new insights into the process-controlled formation of α'- and α-phases were achieved.

CPP 15.15 Mon 18:00 Poster C

Computing thermodynamic and kinetic properties for the primary reactions during sucrose pyrolysis — •Oliver Heymer, Jakob Kraus, and Jens Kortus — Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Str. 23, D-09599 Freiberg, Germany

The thermodynamic properties of the hydrolysis of sucrose as well as the formation of anhydrofructose were investigated at the gold-standard CCSD(T)-level. This level of accuracy enables the comparison of results obtained from perturbation theory and density functional theory. By combining climbing image nudged elastic band calculations with subsequent transition state optimizations, it was possible to report minimum energy paths and highest-energy transition states for both reactions.

At temperatures ranging from 0 to 1500 K, it was found that the hydrolysis reaction is both exothermic and exergonic. For the formation of anhydrofructose, endothermic behavior in the same temperature range was reported. Additionally, this reaction is endergonic from 0 to 450 K and becomes exergonic reaching a temperature of 500 K.

The identification of transition states allowed for an estimate of activation energies and therefore standard reaction rate constants. Lastly, it was possible to study interesting mechanistic aspects that occur during the reactions.

CPP 15.16 Mon 18:00 Poster C

Conformation of star-like molecular brushes with amphiphilic diblock copolymer side arms — •Wenqi Xu[1], Laura Fietzke[2], Feifei Zheng[1], Montserrat Roman-Quintero[1], Peiran Zhang[1], Dmytro Soloviov[3], Rainer Jordan[2], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Faculty of Chemistry and Food Chemistry, Technical University of Dresden, Germany — [3]EMBL at DESY, Hamburg, Germany

Poly(2-oxazoline)s are considered versatile platforms for biomedicine thanks to their biocompatibility and rich architectural possibilities. While linear brushes with amphiphilic copolymer sidearms from poly(2-oxazoline)s have been amply investigated, studies on star-like brushes are still scarce. In the present work, we investigate molecular brushes, in which diblock copolymers from hydrophilic methyl(2-oxazoline) and hydrophobic *n*-butyl(2-oxazoline) are grafted onto star-shaped poly(methyl methacrylate) backbones having functionalities ranging from 2 to 5. The size and shape of the star brushes were investigated in dilute aqueous solutions using dynamic light scattering and synchrotron small-angle X-ray scattering. Our results show that the star brushes are ellipsoids whose degree of elongation depends on the functionality and the relative length of the backbone.

CPP 15.17 Mon 18:00 Poster C

Dynamics of Colloidal Hard-Sphere Systems: A Rescaled Mode Coupling Theory Study — •Joel Diaz Maier and Joachim Wagner — Institut für Chemie, Universität Rostock, 18051 Rostock, Germany

Intermediate scattering functions of liquid-like structured suspensions containing model hard-sphere particles are determined by means of static and dynamic light scattering experiments. The structure and short-time dynamics can be quantitatively described by employing multi-component Percus-Yevick integral-equation theory for the structure factors and the $\delta\gamma$-expansion for hydrodynamic functions. Rescaled multi-component mode coupling theory (RMCT) can quantitatively describe the full, experimentally determined collective dynamics across the entire range of volume fractions investigated within the fluid range when the structure factors used for the calculation of the MCT vertices are rescaled to a lower effective volume fraction. Apart from the scaling factor, RMCT provides a parameter-free, correct description for long-time self-diffusion coefficients and the shear viscosity in the limit of small shear gradients.

CPP 15.18 Mon 18:00 Poster C

Binary mixtures of magnetic shape-anisotropic particles: the role of depletant — Margaret Rosenberg[1], •Ekaterina Novak[2], Elena Pyanzina[2], and Sofia Kantorovich[1] — [1]University of Vienna, Vienna, Austria — [2]Ekaterinburg, Russia

The introduction of non-magnetic particles into a dispersion of magnetic soft (or hard) spheres is recognized to promote the phase separation of the system. Our goal is to explore whether a comparable effect exists in binary mixtures of magnetic shape-anisotropic particles. In this paper, specifically, we undertake a theoretical and computational study of systems comprising either ellipsoids or platelets. We scrutinize the microstructure to assess if the introduction of depletants leads to quantitative or qualitative changes in the radial distribution functions, structure factors, orientational correlations, bond order parameters and static magnetic susceptibility. This research has been partially supported by the RSF Grant No. 19-72-10033. Computer simulations were performed at the Vienna Scientific Cluster (VSC-4).

CPP 15.19 Mon 18:00 Poster C

Electrostatic Screening in Highly Concentrated Salt Solutions — •Esther Ohnesorge, Thomas Tilger, and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

Since colloidal dispersions have a significant importance in our daily life, it is of special interest to get a deeper understanding of which interfacial forces govern their stability and how this stability can be tailored.

For aqueous electrolyte solutions, the DLVO theory is a powerful and well-established framework to describe these interactions at low and intermediate ionic strengths. In contrast, the situation at high ionic strength is less understood and the main methods for direct force measurements give inconsistent results. While the surface force apparatus (SFA) provides clear evidence for a reentrant behavior of the double layer repulsion in the highly concentrated regime - termed underscreening - for a wide range of different electrolytes, similar observations weren't possible with the atomic force microscope (AFM) to date. The reason for this fundamental difference is still unclear.

To elucidate the underlying mechanism, we performed colloidal probe AFM (CP-AFM) measurements in different types of salt solutions, close to their solubility limit. As confining surfaces, silica and mica were compared to study the influence of the surface charge density and to bridge the gap between CP-AFM and SFA.

CPP 15.20 Mon 18:00 Poster C

The simulations of structural, thermodynamical, and mechanical characteristics of the mixture of ionic liquid and water using molecular dynamics: example of [bmim]$^+$[PF$_6$]$^-$ ionic liquid — •Mateja Jovanović[1,2], Miljan Dašić[1,3], and Igor Stanković[1] — [1]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia — [2]Institute of Technical Sciences of SASA, K. Mihailova 35/IV, 11000 Belgrade, Serbia — [3]Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo nam. 2, CZ-16610 Prague 6, Czech Republic

We present a study of the structural, thermodynamical, and mechanical properties of an ionic liquid 1-Butyl-3-methylimidazolium hexafluorophosphate [bmim]$^+$[PF$_6$]$^-$ water mixtures. Our simulation setup allows varying parameters of the system: temperature, concentration of ionic liquid, and shear rate of the system. We report significant changes compared to neat water or ionic liquids in the boiling temperature, diffusion coefficient, and viscosity. Even modest molar fractions of [bmim]$^+$[PF$_6$]$^-$ significantly affect the boiling point. The self-diffusion coefficient of water for the system with a lower concentration of ionic liquid is similar to the self-diffusion coefficient of neat water, and it decreases with increasing concentration of ionic liquid. Viscosity is investigated using equilibrium Green-Kubo relation and non-equilibrium molecular dynamics. In both cases, the viscosity coefficient increases with the increasing weight fraction of ionic liquid.

CPP 15.21 Mon 18:00 Poster C

Effect of different network topologies on swelling and mechanical properties of hydrogels — •Somesh Kurahatti, Mariano Brito, David Beyer, and Christian Holm — Institute for Computational Physics, Stuttgart, Germany

Polyelectrolyte gels exhibit larger swelling ratios than their uncharged counterpart because of the interplay between osmotic pressure induced by the dissociated counterions and the larger stretching induced by the self-repulsion of the backbone charges. Changing the charge density or varying the network contraints affects the swelling capacity as well as the mechanical moduli, which can be shown to also exhibit a strong influence on the desalination efficiency. In the current project, we explore the coupling between bulk modulus and equilibrium swelling of the polyelectrolyte hydrogels and their relation with different network architectures, by analysing various hydrogel conformations including different topologies and network defects. We investigate the bulk modulus and equilibrium swelling as a function of strand length under different salt concentrations and ionization degrees, and compare our results to existing scaling theories. As a result we find a universal coupling between these two quantities in different salinity regimes. The universal coupling can be broken by replacing linear polyelectrolyte strands by bottlebrush polyelectrolytes. Our results are helpful to develop a rational design of functional hydrogels.

CPP 15.22 Mon 18:00 Poster C

Concentration dependent pKa-values in mixtures of trimethylamine N-oxide (TMAO) and amino acids — •Julia Keil, Varun Mandalaparthy, and Nico van der Vegt — Department of Chemistry, Technical University, Darmstadt

The stabilizing effect of trimethylamine N-oxide (TMAO) on proteins is known to be pH-dependent. In our investigation of this pH-dependent action, we studied protonation-deprotonation equilibria in mixed systems containing amino acids and TMAO by performing constant pH molecular dynamics simulations at different pH values. We found that the presence of TMAO causes a decrease in the pKa of acidic and basic groups, while the presence of acidic groups increases the pKa of TMAO. The observed changes in acidity and basicity of the titratable groups correlate with the TMAO concentration. Our results thus indicate a coupling between the equilibria of different titratable groups.

We propose a Wyman-Tanford binding model to explain the underlying mechanism of the observed behavior. Based on this, the accumulation of molecules around a titratable group favors the protonation state which is better stabilized by the presence of these molecules. That leads to a shift in the protonation-deprotonation equilibrium of titratable groups and results in a change of the pKa. More concisely, we find a favorable interaction between deprotonated acidic groups and protonated basic groups and an unfavorable interaction between different protonated basic groups to explain the observed changes of pKa values in mixed solutions of titratable groups.

CPP 15.23 Mon 18:00 Poster C

Using the Light Polarization to Control the Properties of Photoresponsive Metal-Organic Frameworks — •Taher Al Najjar, Anemar Bruno Kanj, Chun Li, and Lars Heinke — Karlsruhe Institute of Technology, Karlsruhe, Germany.

Controlling the properties of materials by applying external stimuli such as light is highly desirable for many applications. One promising realization is the incorporating photochromic molecules in the crystalline, nanoporous structure of metal-organic frameworks (MOFs). MOFs are a class of crystalline nanoporous materials with several unique properties because of their tailorable ordered structures and high surface area. Azobenzene molecules, which respond to light stimulations by isomerisation between its thermodynamically stable trans state and the excited cis state, are among the most popular photochromic molecules and can be used to functionalize MOFs. Using MOFs with fluorinated azobenzene moieties have demonstrated applications such as photoswitchable adsorption, membrane separation and ionic conduction. In this poster, a photoresponsive pillared-layer MOF thin film with incorporated fluorinated azobenzene molecules is presented. In addition to the photoisomerization upon unpolarized light of different wavelengths, the effect of the light polarization is explored. It is found that the polarization can be used to selectively isomerize the functional moieties in the MOF and, thus, to modify the material properties. We show that the polarization can be another useful parameter to control the material properties.

CPP 15.24 Mon 18:00 Poster C

Operando study on structure-activity relationship between electrolyte components and electrochemical performance for all-solid-state lithium-ion batteries — •Yingying Yan[1], Liangzhen Liu[3], Yuxin Liang[1], Fabian A.C. Apfelbeck[1], Guangjiu Pan[1], and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]TUM, MLZ, 85748 Garching, Germany — [3]TUM School of Natural Sciences, Chair of Inorganic and Metal-Organic Chemistry, 85748 Garching, Germany

All-solid-state lithium-ion batteries (ASSLIBs) have received extensive attention as one of the most promising power sources for flexible and wearable electronics. However, the practical application of ASSLIBs has been hindered by poor interfacial stability and inferior ionic conductivity. Solid polymer electrolytes (SPEs), as an important component in ASSLIBs, play a crucial role in determining the overall electrochemical properties, specifically for PEO and PEO-based derivatives, because of their superior interfacial compatibility, wide electrochemical windows and high ionic conductivity. Several strategies have been adopted to address the above issues, nevertheless, the SPEs degradation mechanism is still not clear and needs to be further studied.

Therefore, we combined electrochemical characterization and morphological structure characterization to elucidate the structure-activity relationship between the component structure of the electrolyte and the electrochemical performance.

CPP 15.25 Mon 18:00 Poster C

Temperature dependent crystal structure of Ethylene Carbonate — •Lea Westphal[1,2,3], Volodymyr Baran[4], Peter Müller-Buschbaum[1,2], Florence Porcher[3,5], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]MLZ, TUM, Garching, Germany — [3]Laboratoire Leon Brillouin, UMR12 CEA-CNRS, Gif-sur-Yvette Cedex, France — [4]DESY, Hamburg, Germany — [5]ESS, Lund, Sweden

Performance and safety/stability of Li-ion batteries can be improved by joint optimisation of the charge-storing electrode materials and charge transfer-mediating liquid electrolytes. Most of the research on this has been focused on the electrodes, whilst electrolytes are less studied. An important class of solvents used in liquid electrolytes are linear and cyclic carbonates, because of the combination of physical/chemical properties, electrochemical performance and stability in a mixture with two or more solvents together with a lithium salt. Ethylene carbonate (EC), being the only solvent able to provide the protective SEI layer, is present in almost all commercial batteries, mixed with other solvents. [1] After the determination of the crystal structure of EC [2], this contribution presents room temperature data obtained by Neutron Powder Diffraction at SPODI (FRM II), Total Scattering and temperature dependent Powder X-Ray Diffraction data from beamline P02.1 (DESY), showing the structural evolution at different temperatures.

[1] J.-M. Tarascon & M. Armand, Nature 414, 359-367 (2001).

[2] C.J. Brown, Acta Cryst. 7, 92-96, (1954).

CPP 15.26 Mon 18:00 Poster C

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 15.27 Mon 18:00 Poster C

In-situ interface film forming on the high-voltage LiCoO2 cathode by a tiny amount of nanoporous polymer additives — •Ruoxuan Qi[1], Ming Yang[3], Tianle Zheng[1], Ya-Jun Cheng[3,4], and Peter Müller-Buschbaum[1,2] — [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 — [4]College of Renewable Energy, Hohai University, Jiangsu Province, P. R. China

LiCoO2 (LCO) has been proven for extensive commercial applications owing to its high specific capacity and stability. Therefore, there has been considerable interest in further enhancing its specific capacity by increasing the charging voltage. However, single-crystal LCO suffers a significant capacity degradation when charged to 4.5 V due to the irreversible phase transition and unstable structure. Herein, an ultra-small amount (0.5%wt in the electrode) of multi-functional PIM-1 (a polymer with intrinsic microporosity) additive is utilized to prepare a kind of binder-free electrode. PIM-1 can modulate the solvation structure of LiPF6 due to its unique structure, which helps to form a stable, robust and inorganic-rich CEI film on the surface of LCO at a high voltage of 4.5 V. This reduces the irreversible phase transition of LCO, thereby enhancing cyclic stability and improving rate performance, providing new perspectives for electrodes fabrication and improving high-energy-density cathodes.

CPP 15.28 Mon 18:00 Poster C

3D Electrodeposition Porous Cu for Long-cycling Lithium-Metal Batteries — •Lyuang Cheng[1], Zhuijun Xu[1], Tianle Zheng[1], Yingying Yan[1], Ruoxuan Qi[1], Yuxin Liang[1], Fabian A. C. Apfelbeck[1], Yajun Cheng[2], and Peter Müller-Buschbaum[1,3] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Hohai University, 213022 Changzhou, China — [3]TUM, MLZ, 85748 Garching, Germany

Lithium (Li) metal is the ultimate anode for rechargeable batteries. Its high specific capacity (3860 mAh g*1) and low voltage (*3.04 V vs standard hydrogen electrode) warrant optimal cell energy density. However, these anodes rely on repeated plating and stripping of Li, which leads to consumption of Li inventory and the growth of dendrites that can lead to self-discharge and safety issues. To address these issues and problems related to the volume change of these anodes, a number of different porous conductive scaffolds have been reported to create high surface area electrodes on which Li can be plated reliably. While impressive results have been reported in literature, current processes typically rely on either expensive or poorly scalable techniques. Herein, we report a scalable fabrication method to create porous Cu anodes using a one-step electrodeposition process. The areal loading, pore structure, and electrode thickness can be tuned by changing the electrodeposition parameters, and we show the in-situ WAXS images with lithium growth which can help explain the mechanism of dendrites. We also provide a feasible method to fabricate the porous Cu cathodes with different electrodeposition solution concentrations.

CPP 15.29 Mon 18:00 Poster C

Operando study of structure evolution with PEO-LLZTO composite electrolyte in all-solid-state lithium batteries — •Tannu Garg[1], Yuxin Liang[1], and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials Garching , Germany — [2]MLZ, TUM, Garching, Germany

Solid-state lithium batteries are promising for next-generation energy storage due to their potential for high energy density and safety. This proposal focuses on the operando study of the poly(ethylene oxide) (PEO)-LLZTO composite electrolyte in all-solid-state lithium batteries, with a specific emphasis on observing the structure evolution in bias conditions. The composite electrolyte consists of PEO + LiTFSI matrix and inorganic filler Li6.4La3Zr1.4Ta0.6O12 (LLZTO) in varying weight percentages. The study aims to investigate the phase segregation and polymer region shrinkage with increasing LLZTO content. Additionally, it will explore the diffusion behavior of Li+ ions and the generation of interfaces in different composite electrolytes. The proposal also outlines plans for X-ray scattering analysis and charge/discharge cycling of LLZTO to further enhance the understanding of the system. The study will contribute to the ongoing efforts to develop high-performance all-solid-state lithium batteries by providing insights into the behavior and evolution of PEO-LLZTO composite electrolytes under bias conditions.

CPP 15.30 Mon 18:00 Poster C

Use of High-concentration Lithium-ion Electrolyte to Overcome Challenges of High-temperature Lithium Batteries — •Tianle Zheng[1] and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]TUM, MLZ, 85748 Garching, Germany

Lithium secondary batteries (LSBs) have witnessed explosive growth in the last decade. Traditional Li-ion batteries, on the other hand, are severely constrained in high-temperature applications due to the low thermal stability of the electrolyte/electrode interface and electrolyte decompositions in the cell. Herein, we demonstrate a new electrolyte that achieves excellent stable long-term cycling at 100°C, well beyond the typical 60°C limits of normal conventional Li-ion batteries. The highly concentrated lithium oxalyldifluoroborate (LiODFB) is selected as the only lithium salt with a carefully designed high thermal stability solvent group. As a result, this unique high-concentration electrolyte promotes the formation of a stable and inorganic solid electrolyte interface (SEI) layer on the electrode at elevated temperature, leading to improved performance in MCMB/Li and lithium iron phosphate

(LFP)/Li half-cells. Moreover, it achieves reversible capacities of 160 and 350 mA h/g, respectively, with Coulombic efficiencies (CEs) > 99.3%. Subsequently, we further investigate the mechanism of high-concentration electrolytes by molecular dynamics (MD) simulations and XPS characterization techniques, exploring a new way for future high-temperature electrolytes for Li-ion batteries.

CPP 15.31 Mon 18:00 Poster C

Development of a novel type of solid polymer electrolyte for solid-state lithium battery applications based on lithiumenriched PEO/PVP blend polymer — •Mayank Garg[1], Yuxin Liang[1], and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair of Functional Materials, 85748 Garching, Germany — [2]MLZ, TUM, 85748 Garching, Germany

The growing demand for thin, flexible energy storage devices for applications like flexible electronics and wearable technologies has intensified interest in Solid Polymer Electrolyte (SPE) films. These polymer-based batteries offer a promising alternative due to their thin, flexible nature and seamless integration into devices, coupled with costeffectiveness. This study focuses on enhancing the conductivity of SPE films comprising a blend of biodegradable poly(ethylene oxide) (PEO) and poly(vinyl pyrrolidone) (PVP) as the host matrix, with varied lithium bis(trifluoromethane sulfonyl)imide (LiTFSI) dopant salt concentrations. Structural and optical characterization techniques, including Xray diffraction (XRD), differential scanning calorimetry (DSC), Fourier transform infrared spectroscopy (FTIR), UV-Vis spectroscopy, and electrochemical analysis, were employed. Optimized lithium salt concentrations enabled functional device operation at ambient temperatures (20-60°C), with Impedance Spectroscopy revealing enhanced ionic conductivity. Furthermore, the incorporation of small metal additives further improved the ionic conductivity of the battery cell.

CPP 15.32 Mon 18:00 Poster C

Investigation of Li-ion dynamics at Hybrid Electrolyte Interfaces using M.D Simulations — •Gourav Shukla[1], Diddo Diddens[1,2], and Andreas Heuer[1] — [1]Institut für physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster — [2]Helmholtz Instiitute Münster, Corrensstraße 48, 48149 Münster

Several studies have been conducted to develop novel materials for use as electrolytes, aiming to enhance the performance of batteries in terms of ionic conductivity. Although polymers play a predominant role in electrolytes, the superior mechanical stability of solid electrolytes has spurred the development of hybrid electrolytes that combine the best attributes of both phases. In our work, we are investigating the interface between a Li-salt-containing polycaprolactone polymer and LLZO solid electrolyte, using molecular dynamics simulations. Experiments have shown that polycaprolactone (PCL) exhibits better conductivity when grafted onto solid electrolytes in hybrid systems, compared to non-grafted systems. These systems are studied by MD simulations to investigate the polymer structure and ion distribution as well as the dynamics near the interface. Furthermore, we varied the number of grafted polymer chains on the solid surface to compare the behavior of grafted and non-grafted interfaces. Different force field sets for the solid electrolytes have shown considerable impact on Li-ion migration both at the interface and within the solid phase at a constant temperature. Along with the charge scaling of salt ions for faster dynamics, we also explored the ion migration at different grafted and ungrafted regions.

CPP 15.33 Mon 18:00 Poster C

Investigation of Li-ion dynamics at Hybrid Electrolyte Interfaces using MD Simulations — •Gourav Shukla[1], Diddo Diddens[1,2], and Andreas Heuer[1] — [1]Institut für physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster — [2]Helmholtz Instiitute Münster, Corrensstraße 48, 48149 Münster

Several studies have been conducted to develop novel materials for use as electrolytes, aiming to enhance the performance of batteries in terms of ionic conductivity. Although polymers play a predominant role in electrolytes, the superior mechanical stability of solid electrolytes has spurred the development of hybrid electrolytes that combine the best attributes of both phases. In our work, we are investigating the interface between a Li-salt-containing polycaprolactone polymer and LLZO solid electrolyte, using molecular dynamics simulations. Experiments have shown that polycaprolactone (PCL) exhibits better conductivity when grafted onto solid electrolytes in hybrid systems, compared to non-grafted systems. These systems are studied by MD simulations to investigate the polymer structure and ion distribution as well as the dynamics near the interface. Furthermore, we varied the number of grafted polymer chains on the solid surface to compare the behavior of grafted and non-grafted interfaces. Different force field sets for the solid electrolytes have shown considerable impact on Li-ion migration both at the interface and within the solid phase at a constant temperature. Along with the charge scaling of salt ions for faster dynamics, we also explored the ion migration at different grafted and ungrafted regions.

CPP 15.34 Mon 18:00 Poster C

Simulation of pH-Responsive Hydrogel Formation — •David Beyer[1], Peter Košovan[2], and Christian Holm[1] — [1]Institute for Computational Physics, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Department of Physical and Macromolecular Chemistry, Charles University, 128 00 Prague 2, Czechia

Motivated by recent experiments investigating pH-reponsive, electrostatically triggered hydrogel formation (Mons et al., in preparation), we investigate the interaction between permanently charged sulfonate chains and charge-regulating carboxybetaine chains. Through simulations integrating a state-of-the-art Monte Carlo method for charge-regulating systems with a free energy approach, we obtain the potential of mean force between these chains for different pH-values. Our simulations reveal a substantial charge-regulation effect, elevating the stability of the complex to pH-values beyond what the Henderson-Hasselbalch equation would suggest. A comparative study between fully functionalized and 75% functionalized betaines reveals a further significant enlargement of the pH-stability window in the latter scenario. Overall, our simulations provide a comprehensive explanation for the observed stability at much higher pH-values than naively expected, emphasizing the combined impact of these two effects.

CPP 15.35 Mon 18:00 Poster C

Injectable hydrogels from thermoresponsive tri- and tetrablock terpolymers investigated using scattering methods — •Feifei Zheng[1], Pablo Alvarez Herrera[1], Wenqi Xu[1], Eirini Melampianaki[1], Joachim Kohlbrecher[2], Anna P. Constantinou[3], Theoni K. Georgiou[3], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Paul Scherrer Institut, Villigen PSI, Switzerland — [3]Department of Materials, Imperial College London, London, UK

Thermogels are an exciting class of stimuli-responsive materials with many promising applications, e.g. in 3D bioprinting. The mechanical properties in the gel state strongly depend on the architecture of the polymer. Here we address an ABC triblock terpolymer and a BABC tetrablock terpolymer consisting of the hydrophilic OEGMA (A), the hydrophobic BuMA (B), and the thermoresponsive DEGMA (C).The results from dynamic light scattering on dilute solutions indicate that the hydrodynamic radii of the micelles formed by both, ABC and BABC, increase strongly above 25 °C, and the solutions feature a cloud point, i.e. aggregation of the micelles sets in. By small-angle neutron scattering, we found that ABC forms spherical core-shell micelles, that transform into cylinders at high temperatures, and then become a more compact structure upon further heating. In contrast, the core-shell micelles formed by BABC stay spherical and form small fractal aggregates at higher temperatures, that form a less dense network structure in comparison to those formed by ABC.

CPP 15.36 Mon 18:00 Poster C

Photoswitchable Molecules: Impact on Swelling in Thermoresponsive Polymer Films under UV Irradiation — •David P. Kosbahn[1], Julija Reitenbach[1], Morgan Le Dû[1], Lukas V. Spanier[1], René Steinbrecher[2,3], André Laschewsky[2,3], Robert Cubitt[4], Thomas Saerbeck[4], Christine M. Papadakis[1], and Peter Müller-Buschbaum[1,5] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Institut für Chemie, Universität Potsdam, 14476 Potsdam-Golm, Germany — [3]Fraunhofer Institut für Angewandte Polymerforschung, 14476 Potsdam-Golm, Germany — [4]Institut Laue-Langevin, 38000 Grenoble, France — [5]MLZ, TUM, 85748 Garching, Germany

In this study, we investigated the swelling characteristics of p(AzAm-co-DMAm) and p(AzPyAm-co-DMAm) thin films in both isomer states of the photoswitchable molecules azobenzene (Az) and azopyrazole (AzPy). The influence of UV-irradiation on the swelling behavior in water vapor was explored, aiming to control water uptake, expansion, and morphology on the nanoscale. These materials hold promise for applications such as light sensors, photo-actuators, and drug-delivery systems. Utilizing in situ time-of-flight neutron reflectometry measurements with high temporal resolution at the D17 instrument at ILL, we obtained depth-resolved data about the water distribution during swelling, drying, and irradiation in the dry and swollen states. Our results reveal insights into how photoswitchable molecules affect the microscopic properties of thin polymer films.

CPP 15.37 Mon 18:00 Poster C

Phase behavior of thermo- and photoresponsive diblock copolymers for non-invasive schizophrenic switching — •Peiran Zhang[1], René Steinbrecher[2], André Laschewsky[2], Dmytro Soloviov[3], Peter Müller-Buschbaum[1], and Christine M. Papadakis[1] — [1]Technical University of Munich, TUM School of Natural Sciences, Garching, Germany — [2]University of Potsdam, Institute of Chemistry, Potsdam-Golm, Germany — [3]European Molecular Biology Laboratory, c/o DESY, Hamburg, Germany

Stimuli-responsive diblock copolymers (DBCPs) are of interest as carriers due to their change of properties upon exposure to external stimuli, such as temperature and light. In this study, we present the phase behavior of a series of DBCPs comprising thermo-responsive blocks, one of which is functionalized with a photoactive group. Thus, the DBCP will feature a fixed cloud point (CP) due to the singly responsive block and a tunable CP due to the doubly responsive block. This way, the DBCPs can self-assemble in aqueous solution into micelles and inverse micelles, achieving "schizophrenic switching". Dynamic light scattering indicates that all DBCPs under investigation show a single CP in dilute aqueous solution, namely the one of the singly thermoresponsive block. Small angle X-ray scattering reveals that the DBCPs are expanded chains below this CP and are collapsed at temperatures above, forming large aggregates. Switching the photoactive group by UV irradiation does not have an effect on this behavior, which points to a very high CP of the doubly responsive block.

CPP 15.38 Mon 18:00 Poster C

PNIPAM microgel-stabilized aqueous Pickering foams — •Joanne Zimmer, Gaëtan Barth, Luca Mirau, and Regine von Klitzing — Technische Universität Darmstadt, Department of Physics, Soft Matter at Interfaces, Hochschulstraße 8, 64289 Darmstadt

Particle-stabilized foams (Pickering foams) are gaining increasing attention due to their high long-term stability and possible stimuli-responsiveness. Suitable stabilizers for generation of these foams are PNIPAM microgels (MG) as they possess a high adsorption energy at the water-air-interface compared to classical surfactants. In addition, they show a temperature-dependent reversible volume phase transition which allows for generation of switchable foams, that can be destroyed on demand.

In this work MG stabilized Pickering foams were generated by sparging gas through a PNIPAM MG dispersion. For this purpose, the Teclis Foam Scan device is used, which measures foam properties like foam volume over time, liquid fraction and bubble size and bubble size distribution. A special focus was set on identifying device and sample parameters for generation of foams with a homogenous bubble size distribution. This is essential for a quantitative comparison of the foam properties and investigation of foam destabilization processes. In addition, it must be noticed, that addition of NaCl to the MG dispersion is required to increase the electrical conductivity and allow for determination of the foam liquid content. Thus, the influence of the NaCl concentration on the foaming properties was also subject of this study.

CPP 15.39 Mon 18:00 Poster C

Consistent description of Electrostatic Interactions in Nano-Confinement: from Ab-Initio to Coarse-Grained Models — •Philipp Stärk[1], Zhiwei Jin[1], Henrik Stooss[1], and Alexander Schlaich[1,2] — [1]SC Simtech, Universität Stuttgart — [2]ICP, Universität Stuttgart

The electrode/electrolyte interface is crucial for applications like energy storage and production or electrocatalysis. To describe the microscopic effects, usually the electronic structure (ESP) problem needs to be solved, strongly restricting the accessible length- and time-scales. We combine ESP calculations with semi-classical models that allow for enhanced grand canonical sampling schemes within atomistic simulations of fluids confined between nano-porous electrodes. We derive coarse-grained models that yield the experimentally relevant information like the differential capacitance from the fundamental properties of the electrode/electrolyte interface. Importantly, using this approach allows us to study systematically the influence of the electrode electronic degrees of freedom on the behavior of the confined fluid.

CPP 15.40 Mon 18:00 Poster C

Friction Measurements of Single Pinning Defects Using Droplet Probe Microscopy — •Diego Cortes[1], Michael Kappl[1], Hans-Jürgen Butt[1], and Tomas Corrales[2] — [1]Max Plank Institute, Mainz, Germany — [2]Universidad Tecnica Federico Santa Maria, Valparaiso, Chile

Friction of drops sliding over solid surfaces depends on several effects. By scaling down the size of drops, dissipation at the contact line becomes more and more dominant and can be isolated from other dissipation processes. Here, we measure the energy dissipation of pico liter drops sliding over hydrophobic surfaces using Atomic Force Microscopy. This novel technique allow us to test the wetting behavior of hydrophobic material on sub-micrometer scale.

CPP 15.41 Mon 18:00 Poster C

Electrochemical potential study of the electric double layer in dynamic wetting of electrolyte drops — •Jamila Rzayeva[1], Manuel Brinker[1,2], and Patrick Huber[1,2] — [1]Institut für Material- und Röntgenphysik, Technische Universität Hamburg, Denickestraße 15, 21073 Hamburg, Deutschland — [2]Deutsches Elektronen-Synchrotron DESY, Center for X-Ray and Nano Science CXNS, 22607 Hamburg, Deutschland

Our study aims to investigate the dynamic variations in electrochemical potential within the electric double layer (EDL) of electrolyte's drops. The behaviour of the EDL is investigated during drying and wetting at the interface of the liquid and a conductive gold surface. Understanding the EDL is paramount for fundamental electrochemical processes, especially in dynamic environments where electrolyte drop changes occur. In this work, besides spontaneous evaporation of the liquid, the drop is also deliberately altered by changing its volume. Here, vitally, the advancing and receeding contact angle impacts both the wetting and the potential. The experiments combine drop shape analyser measurements with open circuit potentiometry to yield a comprehensive picture of the link between electrochemistry and wetting of drops on a conductive surface. All of these measurements are conducted with different types of electrolyte and concentration, while also varying the relative humidity of the surrounding atmosphere.

CPP 15.42 Mon 18:00 Poster C

Core-shell nanoparticles for wet-coated surface-enhanced raman scattering (SERS) application — •Jungui Zhou[1], Yingjian Guo[1,2], Suo Tu[2], Anuradha Bhogra[1], Sarathlal Koyiloth Vayalil[1], Daniel Söderberg[5], Peter Müller-Buschbaum[2,3], Peng Zhang[4], and Stephan V. Roth[1,5] — [1]Deutsches Elektronen-Synchrotron, Hamburg, Germany — [2]Technical University of Munich, Garching, Germany — [3]Heinz Maier-Leibnitz Zentrum, Garching, Germany — [4]Sun Yat-sen University, Guangzhou, China — [5]KTH Royal Institute of Technology, Stockholm, Sweden

Plasmonic nanoparticles (NPs) are extensively used in various applications, in particular, SERS, which has been widely used in viral molecular detection. Virus Raman detection is mainly focused on the detection of viral nucleic acid and bases, but the detection of viral proteins is rare. In addition, there is limited knowledge about the interaction between virus proteins and core-shell NPs. Thus, understanding the relationship between the behaviour of viruses and the Raman signal can lead to the development of advanced NPs for virus detection. Here, spraying water-based cellulose nanofiber (CNF) and core-shell NPs solutions is used for the fabrication of sensors. In-situ small-angle grazing incidence X-ray scattering (GISAXS) technique is used to investigate the self-assembly of CNF and NPs during deposition. After the fabrication of sensors, some measurements will be taken, such as Raman, AFM and XPS et al. Moreover, the relationship between NPs, sensor performance, and virus behaviour is explored and constructed to lay solid foundations for the fabrication of sensors for virus detection.

CPP 15.43 Mon 18:00 Poster C

Knot diagrams for 3-periodic entanglements. — •Toky Andriamanalina[1], Myfanwy Evans[1], and Sonia Mahmoudi[2] — [1]University of Potsdam, Germany — [2]Tohoku University, Japan

Polymers, DNA origami crystals, and many other biological and chemical structures present features of entanglement, arranging in a 3-periodic fashion. As the topology of those structures have influence on their physical properties, some knot invariants have been extended into measures, such as the periodic linking number or the periodic

Jones polynomials, to quantify the entanglement. This project aims to give a new mathematical diagrammatic description based on Knot theory for 3-periodic entangled structures. To do so, we project a unit cell of the structure onto a square with periodic boundaries. To the projected curves, we add crossing information, and we introduce new symbols to capture the periodic boundary conditions of the unit cell. The new diagrams require a set of new moves added to the three usual Reidemeister moves.

CPP 15.44 Mon 18:00 Poster C

The neutron time-of-flight spectrometer TOFTOF and its application to soft condensed matter physic — •Marcell Wolf and Christopher Garvey — Heinz Maier-Leibnitz Zentrum, Technische Universität München, Germany

TOFTOF is a direct geometry disc-chopper time-of-flight spectrometer. A cascade of seven fast rotating disc choppers is used to prepare a monochromatic pulsed beam which is focussed onto the sample by a converging super-mirror section. The scattered neutrons are detected by 1000 He detector tubes with a time resolution up to 50 ns. The detectors are mounted at a distance of 4 m and cover 0.75 sr. The high rotation speed of the chopper system together with a high neutron flux in the wavelength range of 1.4 -14 Å allows free tuning of the energy resolution between 3 meV and 2 μeV. The fast neutron background is suppressed by the s-shaped primary neutron guide. This enables the investigation of weak signals. Here we will discuss the value of neutron spectroscopy for different applications in soft condensed matter physics. We will show different sample environments which can be used for sample manipulation.

CPP 15.45 Mon 18:00 Poster C

Deep learning based method for speeding up the extraction of morphological parameters in GISAXS data — •Shachar Dan[1], Eldar Almamedov[2], Stephan V. Roth[1,3], Matthias Schwarzkopf[1], Sven J. Wöhnert[1], Andre Rothkirch[1], and Volker Skwarek[2] — [1]DESY, Hamburg, Germany — [2]HAW, Hamburg, Germany — [3]KTH, Stockholm, Sweden

In situ grazing incidence small angle X-ray scattering (GISAXS) is a powerful tool for accessing nanoscale structure formation in real time with high time resolution and high statistical relevance. Nevertheless, the analysis is clearly time consuming and challenging task, necessitating the need for strategies to speed up the process. In this context we introduce our two-step method that incorporates a pre-processing of GISAXS simulations, which are employed to train a neural network (NN). The NN is subsequently utilized to predict the average cluster radius and distance of the model system gold on silica. There are multiple aspects of the method that require detailed characterization. Here we focus on the effects of using intensity thresholds in the pre-processing step and on the relationship between the network architecture and the distribution of results. As part of ongoing research, we are investigating different configurations and examining their direct impact on the predictive capabilities of the NN. This iterative refinement process aims not only to improve the effectiveness of the approach for the specific system, but also to lay the foundation for its applicability to broader material systems in the field of GISAXS data analysis.

CPP 16: Modeling and Simulation of Soft Matter II

Time: Tuesday 9:30–13:00 Location: H 0106

CPP 16.1 Tue 9:30 H 0106

pyMBE: the Molecule Brewer for ESPResSo — Paola B. Torres[1], •David Beyer[2], Sebastian P. Pineda[3], Peter Košovan[3], and Pablo M. Blanco[4] — [1]Grupo de Bionanotecnologia y Sistemas Complejos. Infap-CONICET & Facultad Regional San Rafael, Universidad Tecnológica Nacional, 5600 San Rafael, Argentina — [2]Institute for Computational Physics, University of Stuttgart, D-70569 Stuttgart, Germany — [3]Department of Physical and Macromolecular Chemistry, Charles University, 128 00 Prague 2, Czechia — [4]Department of Physics, NTNU - Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

We introduce pyMBE (gitlab.com/blancoapa/pyMBE), a Python-based molecule brewer designed for ESPResSo. pyMBE provides a suite of tools aimed at streamlining the construction of coarse-grained representations for molecules characterized by complex architectures, such as polyelectrolytes, peptides, and globular proteins within the ESPResSo molecular dynamics software. Notably, the tool focuses on automating the setup and simulation of chemical reactions in charge-regulating systems, i.e. ionic soft matter with weak acid/base groups. To accommodate a broad range of systems, pyMBE supports chemical reactions in different ensembles, such as constant-pH and grand-reaction. The versatility of the software is exemplified through three practical applications: weak polyelectrolytes in dialysis, charge-regulating peptides, and globular proteins.

CPP 16.2 Tue 9:45 H 0106

Flat-histogram Monte Carlo: algorithm parameters optimization and application extension — •Timur Shakirov — University of Halle, Halle, Germany

Recent developments in flat-histogram Monte Carlo sampling methods have notably expanded our possibility of studying complex physical systems. Despite their decades-long history and established convergence, the problem of optimal parameter selection and the relation between different flat-histogram techniques like Stochastic Approximation Monte Carlo (SAMC) and Multicanonical sampling (MUCA) still present uncharted areas of research. This study proposes general principles for optimizing parameter selection in SAMC, revealing that the optimal convergence achievable is similar to that of MUCA. A significant advancement could be reached by the combination of importance sampling with SAMC or MUCA algorithms, which effectively minimizes the impact of algorithm parameters on the accuracy of estimations. This improvement not only enhances the stability and reliability of simulations but also facilitates an expanded exploration of model parameters within a single flat-histogram simulation run. For example, this approach allows for a more detailed analysis of roles of different energy contributions and enables the estimation of pressure in isochoric Monte Carlo simulations without the need for force or virial computations.

CPP 16.3 Tue 10:00 H 0106

MAICoS: A toolkit for the Molecular Analysis of Interfacial and Confined Systems — •Henrik Stooss[1], Philip Loche[2], Adyant Agrawal[3], Maximilian Becker[4], Kira Fischer[3], Simon Gravelle[5], Marc Sauter[3], Philipp Stärk[1], Srihas Velpuri[1], and Alexander Schlaich[1,3] — [1]SC SimTech, University of Stuttgart — [2]COSMO, EPFL — [3]ICP, University of Stuttgart — [4]Fachbereich Physik, FU Berlin — [5]LIPhy, Université Grenoble Alpes

MAICoS (Molecular Analysis for Interfacial and Confined Systems) is an open-source object-oriented toolkit written in Python tailored to analyse the structural and dynamic properties of interfacial and confined environments derived from molecular simulations. It provides a versatile suite capable of extracting density, orientation, dielectric profiles, structure factors and transport properties from trajectories from a variety of molecular simulation software packages.

The strength of the toolkit lies in its modular design philosophy, which allows analysis in cartesian, cylindrical or spherical coordinates. The use of generic weighting functions extends the adaptability and utility of this software package and illustrates its flexibility and applicability in a wide range of systems. This comprehensive approach facilitates comparative analyses that would prove difficult without a standardised framework. The contribution of MAICoS lies not only in its analytical capabilities, but also in promoting a consistent and interoperable platform for the advancement of FAIR workflows. Furthermore, users can use the framework with tested basic classes to rapidly implement their own robust workflows.

CPP 16.4 Tue 10:15 H 0106

Classical and Quantum Molecular Dynamics to Study Open Molecular Systems — •Sara Panahian Jand and Luigi Delle Site — Institute for Mathematics, Freie Universität Berlin, Germany

Open systems that exchange particle and energy with the environment represent a major challenge for theoreticians. Recently, a model has been derived for a system of molecules that continuously, in a dynamical fashion, exchanges energy and particles with the reservoir considering the physical consistency [1]. The idea is based on the Grand Canonical description of a small open subregion treated at high resolution embedded in a large mean-field reservoir. This has been implemented in the latest version of the adaptive resolution scheme (AdResS). As an example, in order to reach a higher efficiency in treating the nuclear quantum effects, the molecular resolution has been switched from being treated by path integral molecular dynamics (PIMD) with high number of degrees of freedom to a non-interacting point particles. Additionally, the quantum effects manifested as delocalization of hydrogen atoms in the aggregation process of two Fullerene molecules have been studied [2]. In a further step, the aforementioned computational protocol has been extended to couple an open quantum system of molecules with a classical environment. The exchange of molecules between QM and MM region occurs under principles based on physical consistency at macroscopic level and at (microscopic) electronic level [3].

References: [1] L. Delle Site, et al., J. Math. Phys., 61, 8 (2020). [2] S. Panahian Jand, et al., Front. Chem., 10 (2022). [3] L. Delle Site, Comput. Phys. Commun., 222 (2018).

CPP 16.5 Tue 10:30 H 0106

Physical model for magneto-mechanical behavior of magneto-active cylinders — •Mehran Roghani[1], Dirk Romeis[1], Gašper Glavan[2], Inna A. Belyaeva[2], Mikhail Shamonin[2], and Marina Saphiannikova[1] — [1]Institute Theory of Polymers, Leibniz-Institut für Polymerforschung Dresden e. V., Dresden, Germany — [2]East Bavarian Centre for Intelligent Materials (EBACIM), Ostbayerische Technische Hochschule (OTH) Regensburg, Regensburg, Germany

Magneto-Active Elastomers (MAEs) are adaptive composites made of a soft elastomeric matrix with embedded magnetizable micro-particles. Magnetic interactions among the particles enable remote deformation and active modifications of mechanical properties under external magnetic field. This study presents a physically-based model for cylindrical MAE samples that unifies two scales. We use dipolar mean field approach for taking into account the magnetic interactions at micro- and macro-scale. A penalty term is added to the elastic energy due to particle restructuring within the elastomeric matrix. The restructuring causes initially isotropic material to become more and more anisotropic as the magnetic field increases. This transition is taken into account with a transversely isotropic Neo-Hookean material model. The resulting model enables us to explore how microstructure evolution influences the mechanical and magnetic behavior of MAE samples. The model predictions are verified against experiments conducted with different particle volume fractions. The study emphasizes the crucial role of microstructure evolution in modeling MAE deformation, magnetization, and stiffness.

CPP 16.6 Tue 10:45 H 0106

Mixed-Resolution Force Probe Simulations — Marco Oestereich, Jürgen Gauss, and •Gregor Diezemann — Department Chemie, Johannes Gutenberg-Universitaät Mainz, Duesbergweg 10-14, 55128 Mainz, Germany

Force probe molecular dynamics (FPMD) simulations are a well-established technique to investigate the conformational transitions in complex molecular systems. In a standard version of these simulations one end of the molecule is fixed in space and the other end is pulled apart with a constant velocity, very similar to the experimental protocols of dynamic force spectroscopy. In order to overcome the problem that the pulling velocities accessible in simulations are much larger than those in experiments usually coarse-graining (CG) methodologies are used to speed up FPMD simulations. In order to keep atomistic resolution for the solute allowing for a detailed investigation of conformational kinetics we apply the adaptive resolution scheme (AdResS) in our study. In this scheme the solute and the solvent within a well-defined spherical region are treated in an all-atom (AA) manner. Between this region and a CG region outside there is a hybrid region which allows for switching between the two resolutions. We have shown earlier that this setup works well provided the AA region is large enough and the interactions in the CG region are treated via an iterative Boltzmann inversion procedure(1). We present results for two systems undergoing conformational transitions and demonstrate that also a treatment of the CG part of the system employing an ideal gas approximation works extremely well.

30 min. break

CPP 16.7 Tue 11:30 H 0106

Exploring the Role of Ionic Liquids in Polyethylene Terephthalate Glycolysis by Molecular Dynamics Simulations — •Mohamed Nosir and Manuel A Ortuño — CIQUS, Universidad de Santiago de Compostela, 15782 Santiago de Compostela, Spain

Recently, ionic liquids (ILs) have been used as environmentally friendly catalysts in the depolymerization of polyethylene terephthalate (PET). We hereby introduce a computational study to understand the function of ILs as a catalyst in the chemical recycling of PET in the presence of ethylene glycol (EG). Our study focuses on the investigation of the roles of cholinium phosphate $([\mathrm{Ch}]^{+})_3$ $[\mathrm{PO}_4]^{3-}$ IL in the glycolytic degradation of PET. For this issue, classical molecular dynamics (MD) simulations were performed to analyze the structure and thermodynamic properties of the IL/EG/PET ternary systems, under a wide range of experimental conditions. After the equilibration of the system, our MD simulation results provide insights into the potential mechanism of PET glycolysis catalyzed by ILs. Our findings demonstrate that anions are primarily responsible for establishing significant hydrogen bonding with EG. Meanwhile, cations interact with the carbonyl oxygen of PET. Our MD simulations exhibit remarkable agreement with the most recent theoretical and experimental investigations. The employed approach for MD simulation in this particular investigation has the potential to be expanded upon in order to explore additional systems consisting of ILs, alcohols, and PET. As a result, valuable knowledge can be gained regarding the underlying mechanism and kinetics of PET depolymerization.

CPP 16.8 Tue 11:45 H 0106

Universal pairwise interatomic van der Waals potentials from dipolar polarizabilities and C_6 dispersion coefficients — •Almaz Khabibrakhmanov, Dmitry Fedorov, and Alexandre Tkatchenko — Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg

van der Waals (vdW) interactions play an essential role in determining the structure and properties of many molecular and solid-state systems. Classical force fields used in simulations of large systems still mostly rely on empirical Lennard-Jones (LJ) description of vdW interactions. However, LJ potentials are usually prone to large errors and lack physics behind. Therefore, universal and accurate yet non-empirical vdW potentials are strongly desired. Here, we derive the analytical pairwise vdW-QDO potential between atoms, which depend just on two *non-bonded* atomic parameters: static dipole polarizability α_1 and dispersion coefficient C_6. This makes our potential universal, i.e. applicable to all chemical elements.

Our vdW-QDO potential, based on the coarse-grained quantum Drude oscillator (QDO) model for electronic response, shows excellent accuracy for noble-gas dimers against state-of-the-art *ab initio* and analytical methods. In addition, we demonstrate that the vdW-QDO potential can accurately describe group II atomic dimers. We also apply the vdW-QDO potential to small organic molecules and layered materials. We show that the overbinding error increases with the system size, which emphasizes the growing importance of many-body effects in the extended systems.

CPP 16.9 Tue 12:00 H 0106

Solvation Shell Thermodynamics of Extended Hydrophobic Solutes — •Madhusmita Tripathy[1], Swaminath Bharadwaj[1,2], and Nico van der Vegt[1] — [1]Department of Chemistry, TU Darmstadt, Darmstadt, Germany 64297 — [2]Department of Chemical Engineering, Shiv Nadar University, Delhi-NCR, India 201314

Interfacial solvent density fluctuations play an important role in hydrophobic effects, which regulate the functional characteristics of a wide variety of soft matter systems. The loss of water hydrogen bonds near large non-polar solutes leads to enhanced density fluctuations, which make their hydration shells susceptible to small perturbations. Cosolutes can regulate the solute's hydration behavior by enhancing/quenching these fluctuations. To understand the underlying molecular mechanisms, we employ computer simulation to investigate the effect of two adsorbing cosolutes, urea and methanol, on the interfacial thermodynamics of a model extended hydrophobic solute. We find that urea accumulation quenches the interfacial fluctuations, leading to a decrease in the solvation shell compressibility, while methanol accumulation enhances the fluctuations, leading to an increase in compressibility[1]. Analyses on solvation shells energetics indicates that the effect of these adsorbing cosolutes on the density fluctuations, and thereby the stability of the solvation shell, is strongly coupled to their hydration behavior. The observations from this simple model can be discussed in the context of cosolute induced swelling and collapse of

polymers in aqueous solutions.
1. M. Tripathy et al. *J.Chem.Phys.* **2022**, 156, 164901

CPP 16.10 Tue 12:15 H 0106

Thermal dependence of the hydrated proton and optimal proton transfer in the protonated water hexamer — •Michele Casula[1], Félix Mouhat[2], Matteo Peria[1], Tommaso Morresi[3], Rodolphe Vuilleumier[4], and A. Marco Saitta[1] — [1]IMPMC, Sorbonne Université, CNRS, MNHN, Paris, France — [2]Saint Gobain Research Paris, Aubervilliers, France — [3]ECT*-Fondazione Bruno Kessler*, Trento, Italy. — [4]PASTEUR, École normale supérieure, Paris, France

Water is a key ingredient for life and plays a central role as solvent in many biochemical reactions. However, the intrinsically quantum nature of the hydrogen nucleus, revealing itself in a large variety of physical manifestations, including proton transfer, gives rise to unexpected phenomena whose description is still elusive. Here we study, by a combination of state-of-the-art quantum Monte Carlo methods and path-integral molecular dynamics, the structure and hydrogen-bond dynamics of the protonated water hexamer, the fundamental unit for the hydrated proton. We report a remarkably low thermal expansion of the hydrogen bond from zero temperature up to 300 K, owing to the presence of short-Zundel configurations, characterised by proton delocalisation and favoured by the synergy of nuclear quantum effects and thermal activation. The hydrogen bond strength progressively weakens above 300 K, when localised Eigen-like configurations become relevant. Our analysis, supported by the instanton statistics of shuttling protons, reveals that the near room-temperature range from 250 K to 300 K is optimal for proton transfer.

CPP 16.11 Tue 12:30 H 0106

On temperature and coordination effects in liquid water in Raman and infrared spectroscopies: Fingerprinting vibrational frequencies via molecular dynamics — Rodolphe Vuilleumier and •Ari Paavo Seitsonen — Département de Chimie, École Normale Supérieure, Paris

Water is an ubiquitous liquid that has several exotic and anomalous properties. Despite its apparent simple chemical formula, its capability of forming a dynamic network of hydrogen bonds leads to a rich variety of physics. We study [1] the vibrations of water using molecular dynamics simulations, mainly concentrating on the Raman and infrared spectroscopic signatures. We investigate the consequences of the temperature on the vibrational frequencies, and we enter the details of the hydrogen bonding coordination by using restrained simulations in order to gain quantitative insight on the dependence of the frequencies on the neighbouring molecules. Further we consider the differences due to the different methods of solving the electronic structure to evaluate the forces on the ions, and report results on the angular correlations, isotopic mixtures HOD in H_2O/D_2O and and the dielectric constants in water.

[1] *Vibrational spectroscopies in liquid water: on temperature and coordination effects in Raman and infrared spectroscopies*, Rodolphe Vuilleumier and Ari Paavo Seitsonen; *Condensed Matter Physics* **26**, 30101 (2023); DOI: 10.5488/CMP.26.33301

CPP 16.12 Tue 12:45 H 0106

Impact of Electrolyte Composition on Reorganization Energies — •Souvik Mitra, Diddo Diddens, and Andreas Heuer — Institut für physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster

Reorganization energy plays a pivotal role in Marcus theory, which elucidates the mechanism of electron transfer reactions between redox-active organic molecules such as (2,2,6,6-tetramethylpiperidin-1-yl)oxyl (TEMPO) in different solvents. This theoretical work[1] reveals that the presence of salt enhances the rate of homogeneous charge transfer reactions by amplifying the reorganization energy. Our study reveals a connection between reorganization energy and local solvaion environment surrounding the redox molecule.

This research also underscores the importance of quantum phenomena, including charge delocalization, that contribute to extra stability after redox reactions, a feature not present in conventional classical force fields. As a result, we propose adopting machine learning techniques as a means to reduce reliance on demanding quantum mechanical computations and to accurately estimate reorganization energy in intricate systems.

[1] DOI: 10.26434/chemrxiv-2023-5z186-v2

CPP 17: Charged Soft Matter, Polyelectrolytes and Ionic Liquids I

Time: Tuesday 9:30–13:00 Location: H 0107

Invited Talk CPP 17.1 Tue 9:30 H 0107

Dipole-driven Self-assembly and Dynamics in Solutions of Charged Macromolecules — •Murugappan Muthukumar — University of Massachusetts, Amherst, MA, 01003, USA

Control of self-assembled structures of charged macromolecules in aqueous solutions is vital in myriads of natural phenomena. However, a fundamental understanding of the various phenomena exhibited by charged macromolecules is one of the grand challenges in the domains of living matter, biomimicry, and healthcare. The origin of this challenge lies in the simultaneous occurrence of three long-range forces from electrostatics, topology of polymer connectivity, and hydrodynamics. As a result, charged macromolecules exhibit extraordinary behavior unseen in uncharged molecules. Several of these phenomena can be attributed to the dominance of dipole-dipole interaction over monopole-monopole interaction. We will present basic concepts and address structure, dynamics, and transport in a few systems that include biomolecular condensates, polyzwitterions, and intrinsically disordered proteins.

CPP 17.2 Tue 10:00 H 0107

Solvation Behavior of Elastin-like Polypeptides in Divalent Metal Salt Solutions — •Swaminath Bharadwaj[1,2], Yani Zhao[1], Ryan Myers[3], Paul Cremer[3], and Nico van der Vegt[1] — [1]Technical University of Darmstadt, 64287, Darmstadt, Germany — [2]Shiv Nadar Institution of Eminence, Gautam Buddha Nagar, Uttar Pradesh 201314, India — [3]Penn State University, University Park, PA 16802, USA

We studied the effects of $CaCl_2$ and $MgCl_2$ on the cloud point temperature of two different elastin-like polypeptides (ELPs) sequences. Cloud point measurements of these systems were performed along with molecular dynamics simulations and infrared spectroscopy measurements. Changes in the cloud point for the ELPs in aqueous divalent metal cation solutions were primarily governed by two competing interactions: the cation-amide oxygen electrostatic interaction and the hydration of the cation. In particular, Ca^{2+} cations can more readily shed their hydration shells and directly contact two amide oxygens by forming ion bridges. By contrast, Mg^{2+} cations were more strongly hydrated and preferred to partition towards the amide oxygens along with their hydration shells. Next, the partitioning of the cations was strongly influenced by the presence of triglycine motifs in the ELP sequence. In fact, although the more hydrophilic ELP $V_5A_2G_3$ was salted-out of solution by low concentrations of $MgCl_2$, it was salted-in at higher salt concentrations. By contrast, $CaCl_2$ salted the ELP sharply out of solution at higher salt concentrations because of the bridging effect.

CPP 17.3 Tue 10:15 H 0107

Explaining Giant Apparent pKa Shifts in Weak Polyelectrolyte Brushes — •David Beyer[1], Peter Košovan[2], and Christian Holm[1] — [1]Institute for Computational Physics, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Department of Physical and Macromolecular Chemistry, Charles University, 128 00 Prague 2, Czechia

Recent experiments on weak polyelectrolyte brushes found marked shifts in the effective pKa that are linear in the logarithm of the salt concentration. Comparing explicit-particle simulations with mean-field calculations we show that for high grafting densities the salt concentration effect can be explained using the ideal Donnan theory, but for low grafting densities the full shift is due to a combination of the Donnan effect and the polyelectrolyte effect. The latter originates from electrostatic correlations that are neglected in the Donnan picture and that are only approximately included in the mean-field theory. Moreover, we demonstrate that the magnitude of the polyelectrolyte effect is almost invariant with respect to salt concentration but depends on the grafting density of the brush. This invariance is due to a complex cancellation of multiple effects. Based on our results, we show how the experimentally determined pKa shifts may be used to infer the grafting density of brushes, a parameter that is difficult to measure.

CPP 17.4 Tue 10:30 H 0107

Anions and Cations Affect Amino Acid Dissociation Equilibria via Distinct Mechanisms — •Varun Mandalaparthy, Madhusmita Tripathy, and Nico van der Vegt — Department of Chemistry, Technical University, Darmstadt

Salts reduce the pKa of weak acids by a mechanism sensitive to ion identity and concentration that involves charge screening of the deprotonated state. In our recently published study [1], we utilize constant pH molecular dynamics simulations to understand the molecular mechanism behind the salt-dependent dissociation of aspartic acid (Asp). We calculate the pKa of Asp in the presence of monovalent salts and investigate Hofmeister ion effects by systematically varying the ionic radii. We observe that an increase in the anion size leads to a monotonic decrease in Asp pKa. Conversely, changes in the cation size affect the pKa nonmonotonically, interpretable in the context of the law of matching water affinity. The net effect of salt on Asp acidity is governed by an interplay of solvation and competing ion interactions. Our proposed mechanism is rather general and can be applicable to several problems in Hofmeister ion chemistry, such as pH effects on protein stability and ion effects on soft matter interfaces.

[1] Mandalaparthy V., Tripathy M., van der Vegt, N.F.A., Anions and Cations Affect Amino Acid Dissociation Equilibria via Distinct Mechanisms, J. Phys. Chem. Lett. 2023, 14, 41, 9250-9256

CPP 17.5 Tue 10:45 H 0107

Influence of salt concentration and PSS molecular weight on PSS diffusion constant in PSS/PDADMA multilayers — Annekatrin Sill, •Per-Ole Hilken, and Christiane A. Helm — Institute of Physics, University of Greifswald, 17489 Greifswald, Germany

We determine the diffusion constant D_{PSS} of polystyrene sulfonate (PSS) during the growth of polyelectrolyte multilayer films from poly (diallyldimethylammonium) (PDADMA) and PSS. Quartz crystal microbalance dissipation (QCM-D), AFM, and ellipsometry are used. The molecular weight of PDADMA was kept constant (117 kDa), and the one of PSS (M_{PSS}) was varied between 10 and 64 kDa. At the beginning of film build-up, the film thickness grows exponentially with the number of deposited PDADMA/PSS bilayers. Eventually, a transition to non-exponential growth occurs. From the film thickness at this transition and the adsorption time, the diffusion constant D_{PSS} is determined. Varying the NaCl concentration c (between 0.1 M and 1 M), one finds $D_{PSS} = A \cdot e^{(-\beta \cdot c)}$ with A as a constant. β decreases linearly on the increase of M_{PSS}. We obtain a power law on varying M_{PSS}: $D_{PSS} = B \cdot M_{PSS}^{-\gamma}$, with γ increasing linearly with c and B increasing exponentially. In conclusion, we found equations to predict D_{PSS} for given preparation parameters. In our experiments, the diffusion constant D_{PSS} varied by four orders of magnitude. The dependence of D_{PSS} on adsorption time, PDADMA molecular weight, and post-preparation treatment are discussed.

CPP 17.6 Tue 11:00 H 0107

Constrained Ion Conductivity in Isolated Polymer Aggregates — •Alaa Youssef Amin Hassan and Martin Tress — Peter Debye Institute, Leipzig University, Leipzig, Germany

Technological progress and environmental concerns propel the popularity of portable electronics and electric vehicles, which demand robust and lightweight energy storage solutions. While polymeric electrolytes are attractive materials for that, a low ionic conductivity and high contact resistance limit their potential. To overcome this, a design based on a comprehensive understanding of structure-property relationships at the molecular level is required, which can be gained through nanoscale and finite-size investigations. We present a novel setup based on broadband dielectric spectroscopy with nanostructured electrodes combined with physicochemical surface modification methods to study the ion conductivity of polymer aggregates containing $\sim$ 900 to 14 polyethylene oxide chains chemically attached to separated binding sites on a surface. Significant deviations from bulk conductivity indicate that ions engage in (slower) motion along the chains instead of (faster) inter-chain hopping, which dominates in bulk. This may be a general phenomenon of polymeric ion conductors at interfaces, which would reduce their performance through a significant increase in interfacial resistance and electrode polarization. The results suggest bottle-brush architectures can reduce this effect, making them promising candidates for enhanced polymeric electrolytes for better solid-state electrolyte batteries and ion-conducting fuel cell membranes and possibly even improve permeation in polymeric membranes.

15 min. break

CPP 17.7 Tue 11:30 H 0107

Polymerised ionic liquids in solutions: Conformation and rheology — •Carlos Lopez[1], Atsushi Matsumoto[2], Takaichi Watanabe[3], and Walter Richtering[4] — [1]Materials Science and Engineering Department, The Pennsylvania State University, US — [2]Department of Applied Chemistry and Biotechnology, University of Fukui, Japan — [3]Department of Applied Chemistry, Okayama University, Japan — [4]Institute of Physical Chemistry, RWTH Aachen University, Germany, European Union

We investigate the phase behaviour, solution rheology and scattering properties of a polymerised ionic liquid in over 20 different solvents. The polymer is found to be soluble in aprotic solvents of medium or high polarity, but not in protic solvents (e.g. water or ethylene glycol).

In high dielectric constant solvents, the correlation length scales as $\xi \propto C^{-1/2}$, indicating rod-like local conformations. For solvents with modest dielectric permittivities ($\epsilon \simeq$ 18 - 30), the correlation length scales as $\xi \propto C^{-1/3}$, suggesting a partially collapsed pearl-necklace conformation. We hypothesise that the collapsed conformation arises from the influence of dipolar attraction from condensed counterions. In THF ($\epsilon = 8$), the scattering pattern follows the Ornstein-Zernike pattern, similar to neutral polymers.

Viscosity data display the exponents predicted by the scaling theory of Dobrynin et al. However, the ratio $\eta_{sp}/(C\xi^3)$ depends on the solvent type, in contradiction to the scaling model. Our results provide a framework to understand the influence of electrostatics and solvation forces on the structure of polyelectrolytes.

CPP 17.8 Tue 11:45 H 0107

Water harvesting by thermoresponsive ionic liquids — •Robin Cortes-Huerto[1], Nancy C. Forero-Martinez[2], and Pietro Ballone[3] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Deutschland — [2]Johannes Gutenberg-Universität, Mainz — [3]University College Dublin

Ionic liquids (ILs) whose water solutions are thermoresponsive provide an appealing route to harvest water from the atmosphere at an energy cost that can be accessed by solar heating. IL/water solutions that present a lower critical solution temperature (LCST), i.e., demix upon increasing temperature, represent the most promising choice for this task since they could absorb vapour at night when its saturation is highest and release liquid water during the day. In this talk, we present results for the kinetics of water absorption at the surface and the role of nanostructuring in this process as obtained by atomistic molecular dynamics simulations. We focus on the ionic liquid tetrabutyl phosphonium 2,4-dimethylbenzenesulfonate whose LCST in water occurs at Tc = 36 C for solutions of 50/50 wt % composition. The simulation results show that water molecules are readily adsorbed on the IL and migrate along the surface to form thick, three-dimensional islands. On a slightly longer time scale, ions crawl on these islands, covering water and recreating the original surface whose free energy is particularly low. At a high deposition rate, this mechanism allows the fast incorporation of large amounts of water, producing subsurface water pockets that eventually merge into the populations of water-rich and IL-rich domains in the nanostructured bulk.

CPP 17.9 Tue 12:00 H 0107

Microfabricated Poly (Ionic Liquid) Based Electrochemical Oxygen Sensors for Modified Atmosphere Packaging — •Zoë Siebers, Alexey Yakushenko, Ryan Guterman, Maksim Bahdanchyk, Stefan Popović, Dejan Šegan, Petr Vlasov, and Qiang Wang — FaradaIC Sensors GmbH, Richard-Wagner-Straße 23, 10585 Berlin

The large size and high cost of current state-of-the-art oxygen sensors is the main impediment preventing millions of O_2-sensors entering the Internet of the things (IoT) market. This includes the monitoring of millions of bulk packages of perishable food being transported across the planet under a modified or controlled atmosphere (MAP).

The key to miniaturization and mass fabrication of electrochemical amperometric O_2-sensors is microfabrication. To reach such a goal, new special types of polymerized ionic liquid (poly (ionic liquid), PIL) electrolytes have been developed. These PILs are unique as they maintain high enough ionic conductivity after photopolymerization (up to 5×10^{-5} S/cm (24 °C)) and combine gas sensitivity with photopatternability within a single substance.

With these novel materials, we have developed the first fully microfabricated sensor for electrochemical O_2 sensing. With a size of 2 mm x 2 mm x 1 mm it is > ×100 more compact than commercial sensors.

We show that this sensor can be used to reliably measure O_2 concentrations in the specific conditions found in MAP (0-21 % O_2, $0-95$ % relative humidity). An optimized readout algorithm is introduced to increase signal stability and sensor regeneration.

CPP 17.10 Tue 12:15 H 0107

Dynamics of ions in confinement: tuning the nanoporous metal-organic framework host for ionic liquids — •Anemar Bruno Kanj, Rupal Verma, Micaela Vazquez, Zejun Zhang, Abhinav Chandresh, Modan Liu, Wolfgang Wenzel, and Lars Heinke — Karlsruher Institut für Technologie, Karlsruhe, Germany.

Room-temperature ionic liquids (ILs) are molten organic salts. Studying their dynamic properties under nanoporous confinement, such as in metal-organic frameworks (MOFs), is a crucial aspect of fundamental science and can enhance applications like batteries and supercapacitors. Here, we utilize experiments based on MOF thin films and impedance spectroscopy, combined with molecular dynamics simulations. This provides unique insights into their molecular properties: At low IL loadings, the IL cations and anions drift along the electric field in opposite direction. However, at higher concentrations, the ions in the pores mutually obstruct the pathways, leading to a decrease in mobility. This pore blockage results in non-uniform IL density and ion bunching in obstructed pores. By adding lithium in IL, the presence of lithium prevents the formation of Li-anion dimers and the pore blockage and the collapse in conductivity at elevated IL concentrations. The pore size of the MOF confinement also significantly impacts the ion mobility. Smaller pores hinder passage and cause concentration-dependent mobility, while larger pores have minimal interference. We show that the cut-off pore window size corresponds to the diameter of the IL cation-anion dimer. Therefore, optimizing pore size is critical for achieving highly mobile nanoconfined ILs.

CPP 17.11 Tue 12:30 H 0107

Multiscale modeling of ionic liquids under shear — •Abbas Gholami[1], Sebastian Kloth[2], Zhen-Hao Xu[3], Michael Vogel[2], Kurt Kremer[1], Torsten Stuhen[1], and Joseph F. Rudzinski[1,4] — [1]Max Planck Institute for Polymer Research, Mainz — [2]Institute of Condensed Matter Physics, TU Darmstadt — [3]Center for Data Processing, JGU Mainz — [4]Institut für Physik und IRIS-Adlershof, Humboldt-Universität zu Berlin

Room-temperature ionic liquids (ILs) hold significant promise for various applications thanks to their unique attributes like adjustable physiochemical properties. Molecular Dynamics (MD) simulations provide valuable insights into the behavior of ILs, enhancing our understanding of their properties. Using a coarse-grained representation reduces the computational costs considerably by reducing the intermolecular friction and smoothing the free energy surface while providing detailed information at the molecular level. However, in order to use such models to investigate the transport properties, it is necessary to explore the corresponding time scalings when changing model resolutions.

In this study, the behavior of the C4MIM-PF6 IL is investigated under shear using all-atom and coarse-grained MD simulations. Shearing is introduced accurately utilizing the Lees-Edwards boundary condition while conserving momentum and remaining compatible with periodic boundary conditions. To gain a deeper understanding of the coarse-grained model's behavior under shear, the structure and dynamics of the IL are studied at various shear rates, while assessing the consistency of speed-up factors between the cations and anions.

CPP 17.12 Tue 12:45 H 0107

Effect of Molecular Hydrogen on Surface Tension, Surface Enrichment, and Viscosity of Two Imidazolium-Based Ionic Liquids by Molecular Dynamics Simulations — •György Hantal[1], Arsha Cherian[1], Christian Wick[1], Ziwen Zhai[2], Thomas Koller[2], and Ana-Sunčana Smith[1] — [1]PULS Group, Department of Physics, Interdisciplinary Center for Nanostructured Films, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany — [2]Institute of Advanced Optical Technologies and Thermophysical Properties (AOT-TP), Department of Chemical and Biological Engineering Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany

Ionic liquids (ILs) draw attention for their customizable nature in specific tasks through precise combinations of functionalized cations and anions. In supported catalytic systems, IL films host the catalyst and reactant, aiming for accumulation to enhance yield. Despite hydrogen's significance in industrial processes, its impact on IL properties remains insufficiently explored. This study uses molecular dynamics simulations to elucidate hydrogen's influence on two ILs across temperatures and pressures. Viscosity and surface tensions decrease with rising temperature and hydrogen pressure, which is confirmed experimentally. Simulations reveal hydrogen surface enrichment, which is more significant at lower temperatures and pressures. Structural analysis provides a molecular-level interpretation of these observations.

CPP 18: Organic Electronics and Photovoltaics I

Time: Tuesday 9:30–13:00 Location: H 0110

Invited Talk CPP 18.1 Tue 9:30 H 0110

Via bottom-up synthesis of nanoobjects and nanocomposites towards brain-inspired electronics — •Alexander Vahl — Chair for Multicomponent Materials & Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, Kiel, Germany

The recent rapid developments in artificial intelligence require artificial neural networks with growing complexity, increasingly large training data and steeply rising power consumption bringing contemporary artificial neural networks based on conventional silicon technology to the limits. In contrast, neuron assemblies rely on bottom-up network development in soft matter and continuous stimulus-dependent optimization via dynamic reconfigurations, ultimately achieving an outstanding energy efficiency and robustness. To explore these aspects in brain-inspired electronics, conventional deposition approaches in microtechnology are to be complemented by bottom-up self-organization processes, organic matrices and flexible substrates. This contribution showcases nanoobjects, such as Ag based nanoparticles (NPs) prepared by gas phase synthesis, as interesting building units for brain-inspired electronics on unconventional substrates. Resistive switching is demonstrated for a metal/dielectric nanocomposite with threshold characteristics, directly fabricated onto the apex of conductive AFM cantilevers, as well as for AgAu NPs integrated into sparse, self-organized NP/CNT networks, and also in nanofluids, which are obtained via direct incorporation of Ag NPs into polymer matrices. For highly interconnected NP networks, brain-like avalanches and scale-free switching properties are demonstrated.

CPP 18.2 Tue 10:00 H 0110

Coordination of tetracyanoquinodimethane-derivatives with tris(pentafluorophenyl)borane provides stronger p-dopants with enhanced stability — •Andreas Opitz[1], Ahmed E. Mansour[2,1], Ross Warren[1], Dominique Lungwitz[1], Michael Forster[3], Ullrich Scherf[3], Moritz Malischewski[4], and Norbert Koch[1,2] — [1]Humboldt-Universität zu Berlin — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — [3]Bergische Universität Wuppertal — [4]Freie Universität Berlin

Strong molecular dopants for organic semiconductors that are stable against diffusion are in demand, to enhance the performance of organic optoelectronic devices. In this study, we demonstrate the coordination of TCNQ-derivatives with four $B(C_6F_5)_3$ molecules using a single-step solution mixing process. This results in the formation of bulky dopant complexes, 'FxTCN(N)Q-4[$B(C_6F_5)_3$]', exhibiting higher oxidation strength than the original materials themselves. [1] Optical and electrical transport measurements with the prototypical P3HT confirm the higher doping efficiency of FxTCN(N)Q-4[$B(C_6F_5)_3$] compared to F4TCNQ. Additionally, the bulkier structure of FxTCN(N)Q-4[$B(C_6F_5)_3$] is shown to result in higher stability against drift in P3HT under an applied electric field as compared to F4TCNQ. This simple approach of solution-mixing of readily accessible molecules provides the community with access to enhanced molecular p-dopants.

[1] A.E. Mansour *et al.*, *ACS Appl. Mater. Interfaces* **15** (2023) 46148.

CPP 18.3 Tue 10:15 H 0110

Curious DC-conductivity in supramolecular organics — •Heiko Mager[1], Maximilian Litterst[1], Shyamkumar Vadakket Haridas[2], Max von Delius[2], and Martijn Kemerink[1] — [1]Institute for Molecular Systems Engineering and Advanced Materials, 69120 Heidelberg, University, Heidelberg — [2]Institute of Organic Chemistry, Ulm University, 89081 Ulm

We report the discovery of a surprising DC-conductivity in a group of organic molecules (1) that do not share common properties associated with known organic conductors and semiconductors. The conductivity increases over multiple orders of magnitude when increasing material temperature above room temperature. Increased conductivity at room temperature as well as structural analysis by atomic force microscopy (AFM) and X-ray diffraction (XRD) suggest the supramolecular ordering of the materials under bias application at elevated temperatures plays a crucial role. Long time DC-current measurements allow us to exclude trivial explanations for the observed conductivity, like ionic impurities, electrical double layer formation or degradation. Investigation of multiple molecules with similar structure but key differences in functional groups enables us to find common prerequisites for materials to exhibit this kind of conductivity. Based on these prerequisites together with references to existing literature we formulate a theoretical framework for a possible conductivity mechanism.

CPP 18.4 Tue 10:30 H 0110

Langmuir-Blodgett Prepared PMMA Films For All-Solution-Processed Organic Electronics — •Kirill Gubanov, Christiane Sauer, Fabian Streller, Katharina E. Dehm, Ryan W. Crisp, Dustin Vivod, Dirk Zahn, and Rainer H. Fink — Department of Chemistry and Pharmacy, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

A variety of organic materials properties offers opportunities to explore new applications required for the production of sustainable, flexible and low-cost electronic circuitry. Solution-based preparation of high structural quality organic thin films may offer access to such devices. Previously, we reported on successful fabrication of 2-Tridecyl-[1]benzothieno[3,2-b][1]benzothiophene (C13-BTBT) semiconductor crystalline thin films produced via self-assembly at liquid-liquid interface, and microprinted PEDOT:PSS polymer electrodes applied in Organic Field-Effect Transistors (OFETs) for charge-injection or extraction. Here, we report on preparation of Polymethyl methacrylate (PMMA) dielectric films of superior structural quality in the monolayer and multilayer regime by the Langmuir-Blodgett method and their successful application in OFETs. A combined study of NEXAFS linear dichroism and Molecular-Dynamics simulations revealed a beneficial for charge transport preferential upright standing molecular orientation for vacuum-sublimated C13-BTBT semiconductor monolayer deposited on such PMMA thin films. Combining all preparation steps above, all-solution processed OFETs can be fabricated. Research is funded by the BMBF (contract 05K19WE2) and SolTech initiative.

CPP 18.5 Tue 10:45 H 0110

Asymmetry of Charge Carrier Properties: Effects on Performance of p- and n-channel Organic Field-Effect Transistors — •Yurii Radiev[1], Tobias Wollandt[2], Hagen Klauk[2], and Gregor Witte[1] — [1]Philipps-Universität Marburg, Renthof 7, 35037 Marburg, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany

To leverage the full potential of the electronics based on organic field-effect transistors (OFETs), both p- and n-channel devices of similar performance are required [1]. While p-type organic semiconductors (OSCs) have been long known, environmentally stable OSCs for high-performance n-type OFETs have been synthesized only recently [2]. The analysis of such OFETs revealed that the asymmetry of the charge carrier properties limited the use of n-channel devices: large injection barriers and high susceptibility to trap states significantly reduced the device performance. The contact resistance in particular has been gaining more attention recently, since with high charge carrier mobilities the limiting factor for high-frequency device applications becomes the charge carrier injection at the OSC-electrode interface. In this work we compare various p- and n-channel OFET device structures (based on pentacene, DNTT and PhC_2-BQQDI, respectively) to demonstrate the effects of the charge carrier properties asymmetry on the device performance and to discuss the ways to alleviate them [3].

[1] Klauk, H., *et al.*, *Nature* **2007**, *445* (7129), 745-748.

[2] Okamoto, T., *et al.*, *Science Advances* **2020**, *6* (18), eaaz0632.

[3] Radiev, Y., *et al.*, *Organic Electronics* **2021**, *89*, 106030.

CPP 18.6 Tue 11:00 H 0110

Doping gradients optimize the thermoelectric power factor of a conjugated polymer — •Dorothea Scheunemann[1], Jian Liu[2,3], Mariavittoria Craighero[3], Vandna Gupta[3], Sri Harish Kumar Paleti[3], Emmy Järsvall[3], Youngseok Kim[3], Kai Xu[4], Juan Sebastián Reparaz[4], L. Jan Anton Koster[5], Mariano Campoy-Quiles[4], Martijn Kemerink[1], Anna Martinelli[3], and Christian Müller[3] — [1]Heidelberg University, Germany — [2]Chinese Academy of Sciences, China — [3]Chalmers University of Technology, Sweden — [4]Materials Science Institute of Barcelona, Spain — [5]University of Groningen, The Netherlands

Functionally graded materials (FGMs) that feature continuous changes in doping level have been considered as a tool to improve the overall thermoelectric performance of inorganic semiconductors. For organic semiconductors this method has been little used so far. However, since the conductivity σ and the thermopower α vary strongly with the doping level, it can be assumed that a doping gradient also influences the power factor $\alpha^2\sigma$. Here, we show that even moderate electric fields can generate lateral doping gradients in polymer films doped with F4TCNQ, with suitable gradients achieving up to 8-fold enhancement in power factor. Kinetic Monte Carlo simulations enabled us to understand under which conditions a doping gradient can result in an increase in power factor. Our findings indicate that the FGM concept is (i) a way to improve the thermoelectric performance of not yet optimally doped organic semiconductors, (ii) facilitates the screening of different polymer:dopant pairs as a thermoelectric material.

15 min. break

CPP 18.7 Tue 11:30 H 0110

Influence and Control of Spontaneous Orientation Polarization in Binary Organic Semiconductor Mixtures — •Alexander Hofmann, Albin Cakaj, Patrick Bunk, Prakhar Sahay, Johannes Dworschak, and Wolfgang Brütting — Experimental Physics IV, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Spontaneous orientation polarization (SOP) of polar organic molecules is the driving force for the buildup of a giant surface potential (GSP). It has been shown that in organic light emitting diodes (OLEDs) the GSP inside various layers of the device can have positive or negative effects on the overall device performance. Additionally, the introduction of a GSP to former nonpolar layers is possible using the concept of dipolar doping, which has successfully been applied to enhance device performance [1]. To address the effect of polar layers in more detail, the exact properties of dipolar doped layers as well as the underlying physics of SOP in mixtures have to be understood. We investigate prototypical material combinations to gain insight on the orientation mechanisms governing SOP in those mixtures. Understanding the design rules behind dipolar doping will eventually allow the concept to be applied to organic electronic devices other than OLEDs as well.

[1] Noguchi et al., Adv. Optical Mater. 2022, 10, 2201278; DOI: `10.1002/adom.202201278`

CPP 18.8 Tue 11:45 H 0110

Charge-carrier photogeneration in single-component organic semiconductors via low excitation power triplet-triplet annihilation — •Andreas Sperlich[1], Andrei Stankevych[2], Rishabh Saxena[2], Jeannine Grüne[1,3], Stavros Athanasopoulos[4], Prakhar Sahay[5], Wolfgang Brütting[5], Vladimir Dyakonov[1], Heinz Bässler[6], Anna Köhler[2,6], and Andrey Kadashchuk[2] — [1]Experimental Physics 6, University of Würzburg, 97074 Würzburg — [2]Soft Matter Optoelectronics and Bavarian Polymer Institute, University of Bayreuth, 95448 Bayreuth — [3]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK — [4]Departamento de Física, Universidad Carlos III de Madrid, 28911 Madrid, Spain — [5]Institute of Physics, University of Augsburg, 86159 Augsburg — [6]Bayreuth Institute of Macromolecular Research, University of Bayreuth, 95448 Bayreuth

We investigate the carbazole-based material mCBP-CN, a typical host for TADF OLEDs. Our findings challenge established beliefs by demonstrating efficient charge-carrier generation near the absorption edge. Light-induced ESR and luminescence studies at low temperatures unveil slow carrier accumulation and recombination, indicating shallow trapping. Persistent signals in both techniques suggest a common origin. Photocurrent measurements support bimolecular charge generation, emphasizing the role of triplet-triplet annihilation in creating charge pairs. This work highlights unconventional mechanisms in organic semiconductors, relevant beyond OLEDs, but also for long-persistent luminescence, organic photovoltaics, and photocatalysis.

CPP 18.9 Tue 12:00 H 0110

Comparison of electron affinities in organic semiconductors measured by cyclic voltammetry, conventional inverse photoelectron spectroscopy, and low-energy inverse photoelectron spectroscopy — •Mihiro Kubo[1] and Hiroyuki Yoshida[1,2] — [1]Chiba University, Chiba, Japan — [2]Chiba University MCRC, Chiba, Japan

The electron affinity (A) of an organic semiconductor is an essential energy parameter representing the electron transport level. Although A in solid can be determined by inverse photoelectron spectroscopy (IPES), A is often estimated from the reduction potential (E_{red}) measured in solution by cyclic voltammetry. However, because previous IPES data have errors of about 0.3-0.5 eV due to sample damage and low energy resolution, the correlation between E_{red} and A is uncertain. With the development of low-energy inverse photoelectron spectroscopy (LEIPS)[1], the precision of A better than 0.1 eV became possible. In this work, we establish a new correlation using LEIPS data $A=(1.24\pm0.07)*eE_{red}+(5.06\pm0.15)$ eV[2]. In practice, the slope of the correlation is almost similar and A values calculated from this work and previous work differ by less than 0.2 eV over the whole range, although the accuracy of each A should be much higher in LEIPS. Therefore, we further discuss the relationship between the A determined by conventional IPES and LEIPS in terms of energy resolution, sample damage, and vacuum level determination. [1] H. Yoshida, Chem. Phys. Lett., 539-540, 180 (2012); [2] M. Kubo, H. Yoshida, Org. Electron., 108, 106551 (2022).

CPP 18.10 Tue 12:15 H 0110

Tuning programmable luminescent tags by phosphorescent emitter design — •Uliana Tsiko, Heidi Thomas, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden

Purely organic materials with pronounced room temperature phosphorescence (RTP) offer extended emission lifetimes as well as solution processability, mechanical flexibility, and low ecological footprint. These characteristics have led to the development of programmable luminescent tags (PLTs), which allow minimalistic and powerful reusable information storage and labeling [1,2]. To extend the applicability of this technology, emitters with improved RTP efficiency covering a wide spectral range are required.

In our contribution, we present the synthesis as well as the spectroscopic and theoretical analysis of a set of donor-acceptor-donor (D-A-D) materials. Thianthrene as donor unit is combined with nitrogen-containing heterocycles with systematically increasing accepting character. The materials cover a wide range of properties from pronounced fluorescence without RTP to relatively efficient RTP emission but almost no fluorescence. Based on the latter compound, improved PLTs are designed and characterized. Our results provide further insights on structure-property-relationships of RTP emitters strengthening their rational design.

[1] Gmelch et al. Sci. Adv. (2019).

[2] Gmelch et al. Adv. Sci. (2021).

CPP 18.11 Tue 12:30 H 0110

On the decisive influence of surface energy on crystal orientation in films of polythiophenes — •Oleksandr Dolynchuk[1], Robert Kahl[1], Florian Meichsner[2], Alexander Much[1], Mukundan Thelakkat[2], and Thomas Thurn-Albrecht[1] — [1]Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Germany — [2]Applied Functional Polymers, University of Bayreuth, Germany

Semiconducting polymers are an appealing class of functional materials with diverse applications in electronics. Understanding and controlling the crystal orientation in semiconducting polymers is critical to optimizing their efficiency and has long been a major challenge. Using substituted polythiophenes as model semiconducting polymers, it is shown that interfacial interactions at the substrate and vacuum interfaces determine the crystal orientation formed in films of polythiophenes during crystallization from the melt. Namely, we gradually increase the surface energies of the edge-on crystals formed at the vacuum interface by attaching various polar groups at the end of the polymer side chains. As a result, a uniform face-on crystal orientation induced by graphene is achieved in films of the polythiophene with the most polar end group as thick as 200 nm. The face-on crystal orientation is formed in the modified polythiophenes crystallized even on the amorphous surfaces, but by a different growth mechanism. Furthermore, we show that the crystal orientation can be switched in the same sample depending on the crystallization conditions if the competition of interfacial interactions at both interfaces is present.

CPP 18.12 Tue 12:45 H 0110

Systematic search for novel organic ferroelectric materials — •Maximilian Litterst[1], Manjunath Balagopalan[2], Ramon Jannasch[1], Elin Dypvik Sødahl[2], Ola Nilsen[2], Carl Henrik Gørbitz[2], Kristian Berland[2] und Martijn Kemerink[1] — [1]IMSEAM, Heidelberg University — [2]Department of Chemistry, Norwegian University of Life Science, Oslo

Piezo- and ferroelectric materials are forming a multi-billion-dollar market due to their wide applications as actuators, ultrasound generators, mechanical sensors and small-scale energy generators. The market is currently dominated by inorganic materials, which show excellent performance but their application, especially in biological environments, is limited by drawbacks like toxicity, rigidity and acoustic impedance mismatch. Organic ferroelectrics could overcome these limitations. However, the currently most used material PVDF has other limitations including a high coercive field.

Building on previous theoretical work to systematically identify new candidates for ferroelectric materials[1], we employed a combination of experimental techniques to search for signatures of ferroelectricity in these materials. Specifically, we used dielectric relaxation spectroscopy, double wave measurements and CV- measurements. Here, we present an overview over the results of this approach, where several of the investigated materials show clear indications of ferroelectric behavior, highlighting the validity of the approach. At the same time, other materials show intriguing, but so far inconclusive behavior.

[1] arXiv:2306.07138 [cond-mat.mtrl-sci]

CPP 19: Energy Storage and Batteries II

Time: Tuesday 9:30–12:45 Location: H 0111

CPP 19.1 Tue 9:30 H 0111

Reactive molecular dynamics simulations of Lithium-ion battery electrolyte degradation — •Youssef Mabrouk[1], Diddo Diddens[2], and Andreas Heuer[3] — [1]Forschungszentrum Jülich GmbH, Helmholtz-Institute Münster (IEK-12), Corrensstraße 46, 48149 Münster, Germany — [2]Forschungszentrum Jülich GmbH, Helmholtz-Institute Münster (IEK-12), Corrensstraße 46, 48149 Münster, Germany — [3]Institute of Physical Chemistry, University of Münster, Corrensstrasse 28/30, 48149 Münster, Germany

The development of reliable computational methods for novel battery materials has become essential due to the recently intensified research efforts on more sustainable energy storage materials. Here, we use a recently developed framework allowing to consistently incorporate quantum-mechanical activation barriers to classical molecular dynamics simulations to study the reductive solvent decomposition and formation of the solid electrolyte interphase for a graphite/carbonate electrolyte interface. We focus on deriving condensed-phase effective rates based on the elementary gas-phase reduction and decomposition energy barriers. After a short initial transient limited by the elementary barriers, we observe that the effective rate shows a transition to a kinetically slow regime influenced by the changing coordination environment and the ionic fluxes between the bulk electrolyte and the interface. We also discuss the impact of the decomposition on the ionic mobility. Thus, our work shows how elementary first-principles properties can be mechanistically leveraged to provide fundamental insights into electrochemical stability of battery electrolytes.

CPP 19.2 Tue 9:45 H 0111

Design, fabrication and nano-scale characterization of novel SEI layers — •Zhuijun Xu[1], Guangjiu Pan[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, CAS, Ningbo, 315201, China — [3]TUM, MLZ, 85748 Garching, Germany

Lithium has a high specific capacity of 3860 mAh/g and a low electrochemical potential (-3.04 V), promising a high energy density lithium metal battery (LMB). However, the growth of lithium dendrites during charging and discharging would penetrate the separators in LMBs, which leads to short circuits. To inhibit the growth of lithium dendrites, we focus on optimizing the SEI layer through synergetic additives (FEC & LiNO3) in commercial carbonate electrolytes.

In the traditional carbonate electrolytes consisting of ethylene carbonate, dimethyl carbonate, lithium hexafluorophosphate, lithium bis (fluorosulfonyl)imide, the types and contents of the additives (FEC & LiNO3) are precisely regulated. We probe the electrochemical performance and morphology via gGalvanostatic tests and with scanning electron microscopy. Compared the control sample, Li-Li symmetrical cells, Li-Cu cells and Li-Ni83(LiNi0.83Co0.05Mn0.12O2) with the synergetic additives display a better electrochemical performance with smoother surface of lithium metal.

CPP 19.3 Tue 10:00 H 0111

Maximizing utilization of n-type redox sites in polyaniline copolymer for stable non-aqueous sodium/potassium-ion batteries — •Chengzhan Yan, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany.

Polyaniline (PANI) plays a multifaceted role in energy storage because of its tunable composition, structure and morphology. In non-aqueous sodium/potassium-ion batteries, PANI is a prime organic cathode with p-type anion storage. However, its specific capacity is limited owing to the partial utilization of the chain and is of ease decay in changeable electrochemical environments. Moreover, n-type redox sites that coexist with the p-type sites have not received much attention because they are difficult to introduce by in situ chemical oxidation. To this end, the elucidation of n-type reaction in PANI chain and its practice are urgently needed. Herein, a series of carboxylated polyaniline copolymers (named PA2A) are synthesized with a high proportion of quinoid nitrogen. PA2A delivers a high specific capacity of more than 300 mAh/g at a low current density. To further improve the rate performance, PA2A is post-treated by ammonia to achieve a self-doped chain structure (named PA2A-de). This structure greatly accelerates the n-type reaction kinetics, and a low-carboxylated PA2A-de has a high capacity retention of over 70% as the current density increases 20 times from 0.1 A/g to 2 A/g. Besides, the long lifespan of PA2A-de is proven to be sustained in ether-based electrolytes.

CPP 19.4 Tue 10:15 H 0111

Composite Cathode Materials for Improved Iono-Polymer Aluminium Batteries — •Shuvrodev Biswas, Thomas Köhler, Amir Mohammad, Hartmut Stöcker, and Dirk C. Meyer — Institute of Experimental Physics, TU Bergakademie Freiberg

Aluminium batteries are one significant candidate for “post-lithium” batteries due to their exceptional performance in terms of theoretical capacity and cyclability, as well as the inherent advantages of aluminium metal, such as its good availability and low cost. Nevertheless, mass production is still hindered because of several challenges, such as lack of suitable cathode materials, and electrolytes. In search of a better cathode-electrolyte combination, this study investigates several composites based on 9, 10-phenanthrenequinon (PQ) and different graphite modifications synthesized by melt infiltration as novel cathode materials in combination with iono-polymer electrolytes based on triethylamine hydrochloride, polyamide, and aluminium chloride. The electrochemical analysis shows a significant performance boost of the specific capacity with superior rate capability and life cycle when compared to pure graphite or pure PQ. FTIR spectroscopy results also confirm better stability of the composite cathode than the pure PQ cathode. This research highlights the essential electrochemical features of aluminium batteries and serves as the foundation for a new research route using composite cathodes for improved aluminium battery systems.

CPP 19.5 Tue 10:30 H 0111

Dynamic Structure Evolution of Extensively Delithiated High Voltage Spinel — Nicola Jobst[1], •Neelima Paul[2], Premsyl Beran[3], Marilena Mancini[1], Ralph Gilles[2], Margret Wohlfahrt-Mehrens[1], and Peter Axmann[1] — [1]Zentrum für Sonnenenergie- und Wasserstoff- Forschung Baden-Württemberg, Ulm — [2]Heinz Maier-Leibnitz Zentrum, Technische Universität München, Garching — [3]Nuclear Physics Institute, Czech Republic & European Spallation Source ,Lund

High voltage spinel is one of the most promising next-generation cobalt-free cathode materials for lithium ion battery applications. Besides the typically utilized compositional range of LixNi0.5Mn1.5O4 0 < x < 1 , additional 1.5 mol of Li per formula unit can be introduced into the structure in an extended voltage range upto 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 and 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. During the two-phase reaction from cubic (x < 1) to tetragonal (x > 1) phase at ˜2.8 V, we identified the evolution of a second tetragonal phase with x > 2. Evaluation of neutron diffraction data reveal location of additional lithium ions.

CPP 19.6 Tue 10:45 H 0111

Investigation of Li depth profiles in Si/graphite anodes from Li-ion battery cells via NDP and GD-OES — •Ivana Pivarníková[1,2], Marius Flügel[3], Neelima Paul[1], Antonino Cannavo[4], Giovanni Ceccio[4], Jiří Vacík[4], Peter Müller-Buschbaum[1,2], Margret Wohlfahrt-Mehrens[3,5], Thomas Waldmann[3,5], and Ralph Gilles[1] — [1]TUM, MLZ, Garching, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [3]ZSW, Ulm, Germany — [4]NPI, CAS, Rez, Czech Republic — [5]HIU, Ulm, Germany

The loss of Li inventory is a common aging mechanism in Li-ion batteries. To better understand the underlying reversible and irreversible degradation processes in Si/graphite electrodes, depth-resolved methods need to be used to obtain information on the decomposition products of the Li-containing electrolyte across the electrode thickness. In this work we present two Post-Mortem analytical methods, which can be used to obtain quantified Li depth profiles to depths bigger than 10 μm from the electrode surface, the neutron depth profiling (NDP) and glow discharge optical emission spectroscopy (GD-OES). The validation of GD-OES using NDP by examining the Si/graphite anodes from cylindrical 21700 cells is presented. These two methods are complementary to each other. It has been demonstrated that the preferential sputtering can occur on the anode surface during the GD-OES measurements. This phenomenon is caused by the higher sputter rate of Li, as it is mainly present in the Li plated layer or in the solid electrolyte interface (SEI).

CPP 19.7 Tue 11:00 H 0111

Novel Current Collectors for Post-Lithium Energy Storage Systems using Thin-Film Coating — •Oliver Schmidt, Amir Mohammad, Shuvrodev Biswas, Hartmut Stöcker, and Dirk C. Meyer — TU Bergakademie Freiberg, Leipziger Straße 23, 09599 Freiberg, Germany

An often-overlooked component of batteries is the current collector, which provides the connection between the ionic charge carriers and the electronic current. For post-Lithium batteries like Aluminium-ion batteries the requirements are more demanding than for Lithium-ion batteries. The electrolytes in these batteries are highly acidic ionic liquids based on Aluminium chloride. They tend to corrode conventional current collectors such as Aluminium or Copper.

Stable materials for the current collector are refractory metals such as Mo, conductive TiN or amorphous Carbon. Instead of using these materials directly as foils, they are coated on top of a carrier foil (e.g. Aluminium, Polyimide). To reduce weight and price and to simplify handling, different coating systems are developed. To improve the adhesion and coating properties, a subsequent flash lamp annealing (FLA) is used. The FLA process provides a very rapid annealing step (pulse length of 1 to 10 milliseconds) without damaging the substrate. After an initial optimization of coating thickness and FLA treatment, the obtained coatings are found to be long-term stable and well applicable in Aluminium batteries.

15 min. break

CPP 19.8 Tue 11:30 H 0111

Coexistence of Cationic and Anionic Phosphate Moieties in the Solid Acid $Cs_7(H_4PO_4)(H_2PO_4)_8$ — •Christian Dressler[1], Jonas Hänseroth[2], and Daniel Sebastiani[2] — [1]Theoretical Solid State Physics, TU Ilmenau, Germany — [2]Theoretical Chemistry, MLU Halle-Wittenberg, Germany

We have studied the proton distribution and proton mobility in the recently synthesized solid state proton conductor $Cs_7(H_4PO_4)(H_2PO_4)_8$ by ab initio molecular dynamics simulations.[1] In agreement with experimental observations [2], we can clearly distinguish in our simulations an unusual cationic $H_4PO_4^+$ and an anionic $H_2PO_4^-$ form that coexist in this solid acid. This paradox situation is achieved by partial substitution of Cs^+ by $H_4PO_4^+$ in CsH_2PO_4. Thus, H_nPO_4 act simultaneously as both the positive and the negative ion of the salt. We analyze the dynamical protonation pattern within the unusual hydrogen bond network that is established between the ions. Our AIMD simulations show that a conventional assignment of protonation states of the phosphate groups is not meaningful. Instead, a better description of the protonation situation is achieved by a fractional assignment of the strongly hydrogen-bonded protons to both its nearest and next-nearest oxygen neighbors. Furthermore, we also discuss the effect of the insertion of the cation $H_4PO_4^+$ on the proton mobility.

[1] Dreßler, Hänseroth, Sebastiani, J. Phys. Chem. Lett. 2023, 14, 32, 7249-7255; [2] Wang, Patel, Sanghvi, Hu, Haile, J. Am. Chem. Soc. 2020, 142, 47, 19992-20001.

CPP 19.9 Tue 11:45 H 0111

Operando observation of lithium dendrite growth in polymer based batteries by nanofocus WAXS — •Fabian A.C. Apfelbeck[1], Gilles E. Wittmann[2], Lyuyang Cheng[1], Yuxin Liang[1], Yingying Yan[1], Anton Davydok[3], and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching — [2]MLZ, TUM, Garching — [3]Institute of Material Physics, Helmholtz-Zentrum Hereon, Hamburg

Single-ion conducting polymers are a promising candidate as electrolyte in lithium metal batteries due to a theoretical transference number of one, which is accompanied by the suppression of lithium dendrite growth. This can extend the cycle life and improve the overall saftey of lithium metal batteries. However, the practical usage is still under debate since dendrite growth has also been reported in single-ion conducting polymer based cells. Here, we study operando the lithium dendrite growth in lithium symmetric cells with polymer electrolytes by nanofocus wide angle X-ray scattering (nano WAXS). With this technique, we can spatially resolve the crystalline behavior of the cell on a nanoscale by scanning the polymer during operation.

CPP 19.10 Tue 12:00 H 0111

"Corrections of Cation-pi Interactions in Force Field with $1/r^4$ and Sigma (σ) Nonbonded Terms" — •Diptesh Gayen[1], Yannik Schütze[2], Sebastien Groh[1], and Joachim Dzubiella[1] — [1]Applied Theoretical Physics - Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany — [2]Theoretical Chemistry, Institute of Chemistry and Biochemistry, Freie Universität Berlin, 14195 Berlin, Germany

This study explores cation-π interactions in a poly(4-(thiophene-3-yl) benzenethiol) (PTBT) cathode for Li-S batteries using molecular dynamics (MD) simulations. MD often underestimates cation-π binding energies compared to quantum mechanics (QM). To address this, we enhance the MD force field for PTBT, introducing distance-dependent terms optimized for accurate cation-π representation. The study contributes insights into refining force fields for realistic simulations of polymer-ion interactions in Li-S batteries. Additionally, we construct an MD simulation model for representative PTBT-electrolyte-solvent systems, incorporating LiTFSI and LiNO3 electrolytes in 1,2-dimethoxyethane and 1,3-dioxolane mixtures. Our work provides a pathway to improve the accuracy of MD simulations in studying ion dynamics in polymer-based cathodes, with implications for enhancing Li-S battery performance.

CPP 19.11 Tue 12:15 H 0111

The wavelength-dependent photogeneration and mobility of holes in hematite for photoelectrochemical water splitting — •Yuke Yang, Felix Zerres, Yujin Tong, and Richard Kramer Campen — Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany

Photoelectrochemical water splitting is a promising technique for converting solar energy into hydrogen fuel. It is well-established that a significant percentage of absorbed photons in common photoelectrodes do not contribute to chemical reactions. This effect in oxides is usually attributed to polaron formation and subsequent recombination of some fraction of the excited charge carriers. Methods to directly probe polaron populations are, therefore, an essential part of any materials optimization strategy. Most of these methods are suitable for application only by specialists: they require amplified laser systems and ultrasensitive detection schemes. Here we conduct chopped photocurrent measurements in a hematite(α-Fe_2O_3) photoanode as a function of photon energy. The bias and wavelength dependence of the resulting kinetics, and their change when adding the hole scavenger H_2O_2 to the electrolyte, allow us to characterize electron polarons (that adversely affect device performance) and hole polarons that are OER intermediates. This straightforward way of characterizing polaron energies and relaxation time in this model oxide photoanode offers a useful complementary tool to more complicated experimental techniques that are well matched to high throughput anode creation to empirically changes in polaron stability with changes in catalyst or electrolyte composition.

CPP 19.12 Tue 12:30 H 0111

The Role of Oxygen in Phenazine-TCNQ Charge-Transfer Complex Regeneration — •Kirill Gubanov[1], Yana Reva[1], Daniel Langford[1], Frank Hampel[1], Andreas Späth[1], Evanie Franz[1], Ryan W. Crisp[1], Sebastian Bochmann[1], Benjamin Watts[2], Jörg Libuda[1], Dirk M. Guldi[1], and Rainer H. Fink[1] — [1]Department of Chemistry and Pharmacy, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland

Organic charge-transfer complexes (CTC) are promising candidates as electrode material in rechargeable lithium-ion batteries. Besides being renewable, non-toxic and affordable in contrast with their inorganic counterparts, the intrinsic features of the organic CTC, such as electrical conductivity or high cycle performance, are greatly enhanced in comparison with their single-moiety parent components. However, the charge-trap states, induced by the structural defects within the CTC crystal lattice lower the initial degree of charge transferred from the electron donor to acceptor molecules. Remarkably, oxygen-enriched environment regenerates the charge-transfer process in the complex of Phenazine (PNZ)/Tetracyanoquinodimethane (TCNQ) CTC crystal nanoaggregates. By means of the NEXAFS-based microspectroscopy and (spectro)electrochemical methods, we prove that the oxygen donates electrons to fill the trap states and ultimately enhances the degree of charge-transfer from PNZ to TCNQ, improving the overall charge-transport properties of the material. The research is funded by the BMBF (contract 05K19WE2).

CPP 20: Active Matter II (joint session BP/CPP/DY)

Time: Tuesday 9:30–13:00 Location: H 1028

CPP 20.1 Tue 9:30 H 1028

Disorder-induced cooperative behaviour in aligning self-propelled particle systems — •Eloise Lardet and Thibault Bertrand — Imperial College London, London, UK

In 1995, Vicsek et al. wrote a seminal paper describing a simple model that displays a transition from disorder to collective ordered behaviour. It describes a system of self-propelled point particles that align with their neighbours within a certain radius. This minimal model displays rich nonequilibrium behaviours such as flocking and banding. Inspired by the random couplings of spin glass models, I present numerical findings of introducing Gaussian distributed pairwise couplings into a self-propelled particle system. Through adding further disorder by increasing the standard deviation of the Gaussian distribution that the couplings are drawn from, we are able to observe the emergence of global polar order in systems where the majority of couplings are anti-aligning.

CPP 20.2 Tue 9:45 H 1028

Swarming of self-steering and responsive active particles — •Rajendra Singh Negi, Roland G. Winkler, and Gerhard Gompper — Theoretical Physics of Living Matter, Institute of Biological Information Processing (IBI-5), Forschungszentrum Jülich, 52425 Jülich, Germany

The collective behavior of self-propelled agents emerges from the dynamic response of individuals to various input signals [1,2]. In our model of intelligent active Brownian particles (iABPs), information about the position and orientation of neighboring particles, obtained through directed visual and isotropic perception, respectively, is used to adjust the propulsion direction. The maneuverability due to visual signal and polar alignment determines the self-organization. Several non-equilibrium structures like worms, milling, compact, and dispersed clusters are obtained at different parameter sets [2]. As the strength of polar alignment increased compared to visual maneuverability, worm structures dominate over compact structures. Our results help to understand the collective behavior of cognitive self-propelled particles, like animal herds and micro-robotic swarms.

[1]. R. S. Negi, R. G. Winkler, and G. Gompper, Emergent collective behavior of active Brownian particles with visual perception, Soft Matter **18**, 6167 (2022).

[2]. R. S. Negi, R. G. Winkler, and G. Gompper, Collective behavior of self-steering particles with velocity alignment and visual perception, (2023) arXiv:2308.00670 .

CPP 20.3 Tue 10:00 H 1028

Effect of cell-cell interactions on the collective behaviour of gliding *Chlamydomonas* populations — •Alexandros Fragkopoulos, Justin Nevells, Timo Völkl, and Oliver Bäumchen — University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany

Cilia and flagella represent universal tools enabling cells and microbes to propel themselves in diverse environments. In the case of the unicellular biflagellated microbe *Chlamydomonas reinhardtii*, the flagella are used not only to swim in the surrounding medium, but also to adhere to surfaces. In this adhered state, a second flagella-mediated motility mode is observed, during which the cells glide along the surface. This is achieved by means of force transduction through an intraflagellar transport machinery. We recently showed that gliding *C. reinhardtii* cells form weak clusters, most likely assisted by mechanosensing of their flagella [1]. Here we show that *Chlamydomonas noctigama*, a close relative of *C. reinhardtii*, exhibits significantly stronger cell-cell interactions, resulting in pronounced cell clustering even at low densities. In addition, we observe that *C. noctigama* preferentially attach nearby other cells. Finally, we use morphological tools to quantify and compare the clusters to *C. reinhardtii*. By understanding the changes of the cell-cell interactions between the species, we aim to dissect their contribution to the observed cell clustering.

[1] Till et al., *Phys. Rev. Res.* **4**, L042046 (2022).

CPP 20.4 Tue 10:15 H 1028

Magnetic colloidal crystals activated by light-driven bacteria — •Helena Massana-Cid[1], Claudio Maggi[1,2], Giacomo Frangipane[1], and Roberto Di Leonardo[1,2] — [1]Department of Physics, Sapienza University of Rome, Rome, Italy — [2]NANOTEC-CNR, Institute of Nanotechnology, Rome, Italy

Active solids, or self-propelling units elastically coupled on a lattice, are recently of growing interest and are predicted to show emerging out-of-equilibrium behaviour, while they can inspire the design of numerous applications. We show for the first time an experimental realisation of a large ordered active solid with activity and confinement tuneable in-situ and on-command. This two-dimensional active solid is composed of repulsive magnetic particles activated by a photokinetic bacterial bath. The bacteria induce active motion into the crystal by pushing its particles and, in a simplified picture, this can be described by an equilibrium state with a higher effective temperature. Nevertheless, this framework breaks down qualitatively because of the active fluctuations time correlations due to the persistent motion of bacteria. We explore the emerging dynamics of this active solid for different values of activity, controlled by the applied light, and repulsion strength, determined by the external magnetic field. Furthermore, we show how we can melt the crystal by increasing activity. Our findings pave the way to unveil the properties of a novel out-of-equilibrium system, an active colloidal solid, which presents questions vastly interesting from a statistical mechanics point of view.

CPP 20.5 Tue 10:30 H 1028

Billiards with Spatial Memory — Thijs Albers, Stijn Delnoij, Nico Schramma, and •Mazi Jalaal — Institute of Physics, University of Amsterdam, Amsterdam, The Netherlands

It has been proposed that spatial memory can lead to more efficient navigation and collective behaviour in biological systems. This raises important questions about the fundamental properties of dynamical systems with spatial memory. We present a framework based on mathematical billiards in which particles remember their past trajectories and react to them. Despite the simplicity of its fundamental deterministic rules, such a system is strongly non-ergodic and exhibits highly-intermittent statistics, manifesting in complex pattern formation. We show how these self-memory-induced complexities emerge from the temporal change of topology and the consequent chaos in the system. We study the fundamental properties of these billiards and particularly the long-time behaviour when the particles are self-trapped in an arrested state. We exploit numerical simulations of several millions of particles to explore pattern formation and the corresponding statistics in polygonal billiards of different geometries. Our work illustrates how the dynamics of a single-body system can dramatically change when particles feature spatial memory and provide a scheme to further explore systems with complex memory kernels.

CPP 20.6 Tue 10:45 H 1028

Chemical communication in suspensions of active particles — •Nils Göth and Joachim Dzubiella — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Germany

Chemical communication of bacteria plays an important role in their individual and collective behavior. Here, we study how a simple form of interparticle communication influences a system of colloidal particles. We employ two-dimensional Brownian dynamics simulations of a model of Responsive Colloids, in which the particle size and the internal proton concentration are explicit internal degrees of freedom. The communication between the particles is modeled as a chemical field around each particle to which the other particles respond by changes in their size. We find a rich behavior of structures, including pseudo-regular oscillations and longitudinal waves.

15 min. break

CPP 20.7 Tue 11:15 H 1028

Structural Colour from Collective Gliding Bacteria Motion — •Junwei Wang[1], Marina Portoghese[2], Laura Caton[2], Colin Ingham[3], and Silvia Vignolini[1] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]University of Cambridge, Cambridge, UK — [3]Hoekmine BV, Utrecht, Netherland

We report a type of marine, non-pathogenic, gliding bacteria, Flavobacterium Iridescent 1 (IR1), that grows into a dense active liquid crystal colony, exhibiting structural colour. We demonstrate different crystalline phases arising from collective bacteria motility correlate with varied optical appearances of the colony. We show the hierarchical collective motions of the rod-like bacteria that organize into clusters, monolayer, multi-layers and finally into large scale vortices. We also illustrate how the bacteria colony adapts to confinement of different geometries.

CPP 20.8 Tue 11:30 H 1028

Chiral active molecules in traveling activity waves — •Bhavesh Valecha[1] and Abhinav Sharma[1,2] — [1]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany — [2]Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, 01069 Dresden, Germany

Directed motion is crucial for the survival and maintenance of life-supporting functions of numerous biological systems, e.g., motion of sperms towards the egg during fertilisation or movement of immune cells to fight-off an infection. While systematic studies of chiral active molecules simulating crucial aspects of these systems in stationary activity gradients do exist [1-3], the majority of physical scenarios revolve around activity fields that vary with time. So, in this project we study the simplest possible case of an active molecule, the active dimer, in a propagating activity wave. We show that this simple molecule can show very rich emergent tactic behaviour using a cooperative mechanism between the two active chiral particles. In particular, this dimer can, on average, move along with the wave, against the wave motion or not move at all depending on the magnitude of chiral torque and the wave speed. We believe that this study can provide important insights into the design principles of hybrid bio-molecular devices of the future.

[1] P. L. Muzzeddu, H. D. Vuijk, H. Löwen, J.-U. Sommer, and A. Sharma, J. Chem. Phys. **157**, 134902 (2022)

[2] H. D. Vuijk, S. Klempahn, H. Merlitz, J.-U. Sommer, and A. Sharma, Phys. Rev. E **106**, 014617 (2022)

[3] H. Merlitz et al., J. Chem. Phys. **148**, 194116 (2018)

CPP 20.9 Tue 11:45 H 1028

Physical principles of space allocation in an active biofluid — •Sebastian W. Krauss, Mithun Thampi, Pierre-Yves Gires, and Matthias Weiss — Experimental Physics I, Bayreuth, Germany

Living matter has the remarkable ability to self-organize into distinct cellular entities that ultimately form the building blocks of organisms. The organisation in multi-cellular systems emerges by replicating a single fertilized oocyte as template structure in multiple division cycles. In contrast, recent studies on Xenopus egg extracts have shown that an active biofluid that is devoid of template structures and genetic material can spontaneously self-organize into compartments in an ATP-driven fashion even when protein synthesis is blocked. The emerging compartments (protocells) are distinct, lack a confining membrane envelope, and vanish after all ATP has been consumed. Here, we show that protocell geometry is determined by a random-packing process with a coarse-graining dynamics that is similar to two-dimensional foams [Development 150, dev200851 (2023)]. Protocell sizes are seen to be tunable by altering the dynamics of microtubules while preserving geometric features of the pattern. Confining the self-organizing fluid in ellipsoidal microfluidic cavities, i.e. mimicking natural confinements like those in embryos, pattern formation is seen to adapt to the confinement, exhibiting a surprising similarity to spatial compartmentalization in early embryos. Further, we observe that an increasing aspect ratio of the chamber results in the formation of smaller protocells. Our results indicate that mechanical cues and simple self-organization principles are key ingredients in many developmental processes.

CPP 20.10 Tue 12:00 H 1028

Foams Come to Life — •Ivan Maryshev[1], Filippo De Luca[1,2], and Erwin Frey[1] — [1]Ludwig-Maximilians-Universität München, München, Germany; — [2]University of Cambridge, Cambridge, United Kingdom

Recent experiments on active filament mixtures revealed a new non-equilibrium phase called active foam, consisting of a continuously reconfiguring network of bilayers [1]. The existence of similar structures was previously predicted in phenomenological models [2]. Here we introduce a microscopic model for microtubule-motor mixtures and rigorously derive a hydrodynamic theory that recapitulates the experimental observations. We explain the observed instabilities and associated mechanisms. Finally, we discuss various forms of foam that can be realized in different active matter systems and classify them according to the symmetry and order parameters involved. This research contributes to our understanding of the complex behavior exhibited by active foams and provides insights into their dynamics.

[1] B. Lemma, N. P. Mitchell, R. Subramanian, D. J. Needleman, and Z. Dogic (2022). Active microphase separation in mixtures of microtubules and tip-accumulating molecular motors. Phys. Rev. X 12(3), 031006.

[2] I. Maryshev, A. Morozov, B. Goryachev, and D. Marenduzzo (2020). Pattern formation in active model C with anchoring: bands, aster networks, and foams. Soft Matter 16(38), 8775-8781.

CPP 20.11 Tue 12:15 H 1028

Modelling cancer metastasis with active nematics — •Josep-Maria Armengol-Collado[1], Luca Giomi[1], Oleksandr Chepizhko[2], Stephanie Alexander[3], Esther Wagena[3], Bettina Weigelin[3], Peter Friedl[3], Stefano Zapperi[4], and Caterina A.M. La Porta[5] — [1]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands — [2]Faculty of Physics, University of Viena, Boltzmanngasse 5, Viena, Austria — [3]Department of Medical Biosciences, Sciences, Radboud University Medical Centre, 6525 GA Nijmegen, The Netherlands — [4]Center for Complexity and Biosystems, Department of Physics, University of Milan, via Celoria 16, 20133 Milan, Italy — [5]Center for complexity and Biosystems, Department of Environmental Science and Policy, University of Milan, via Celoria 10, 20133 Milan, Italy

Tumor invasion is characterized by the coordinated movement of cancer cells through complex tissue structures. Here, we focus on recent in vivo experiments where metastasis is observed through the dermis of a living mouse, and low-cohesive modes of collective migration have been identified. Interestingly, local rotational patterns give rise to antiparallel flow tracks that deform the extracellular matrix and establish a sustained flow of cells. To model this phenomenon, we employ the framework of nematic liquid crystals in the so-called "active turbulence" regime. Analysing the effects of confinement and the role of topological defects we provide significant insights to better understand the underlying mechanisms of cancer cell migration.

CPP 20.12 Tue 12:30 H 1028

Flow Localization on Active Ordered Surfaces — •Rushikesh Shinde[1], Raphael Voituriez[2], and Andrew Callan-Jones[1] — [1]Laboratoire de Matière et Systèmes Complexes, Université de Paris Cité and CNRS, Paris, France — [2]Laboratoire de Physique Théorique de la Matière Condensée, Sorbonne Université and CNRS, Paris, France

During morphogenetic processes, active flows occur in the plane of curved tissues. Tissues often exhibit orientational order, and topological defects arise during tissue development. We have studied the behavior of a +1 defect in a film of active ordered fluid on a curved axisymmetric surface. We find strikingly different physics compared with the flat-space variant of the problem, in which extensile activity causes vortex-like or aster-like integer defects to undergo spiral ordering and rotational motion. We focus in particular on the influence of extrinsic curvature in the elastic free energy, usually neglected in theories of ordered fluids on curved surfaces. We consider two biologically-relevant surfaces: a capped-tube-like rigid surface, similar to epithelial tubes; and a bump on an otherwise flat plane. In the first case, we find that the activity threshold for instability becomes independent of system size, and spontaneous rotational flows become localized. In the latter case, we find that an aster can be passively unstable towards a spiral state, and as a result, contractility-driven active flows are thresholdless and localized. High contractility extinguishes the flow and restores the aster. Surprisingly, for high enough saddle curvature, the spiral to aster transition shifts from continuous to discontinuous.

CPP 20.13 Tue 12:45 H 1028

Self-Organization in Quorum-Sensing Active Matter: The Interplay between Nonreciprocity and Motility — •Yu Duan[1], Jaime Agudo-Canalejo[1], Ramin Golestanian[1,2], and Benoît Mahault[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

Over the past years, the generation of interactions breaking action-reaction symmetry has emerged as new paradigm for active matter. The generalization of the Cahn-Hilliard theory of phase separation to nonreciprocal mixtures predicts the emergence of traveling states that break time reversal symmetry when intra-species attraction leads to demixing while chasing inter-species interactions are present. Here, we study a minimal model of active phase separation involving two species of particles regulating their self-propulsion speed via quorum-sensing rules, and identify a mechanism for dynamical pattern formation that does not rely on the standard route of intra-species effective attractive interactions. Instead, our results reveal a highly dynamical phase of chasing bands induced only by the combined effects of self-propulsion and nonreciprocity in the inter-species couplings. Turning on self-attraction, we find that the system may phase separate into a macroscopic domain of such chaotic chasing bands coexisting with a dilute gas. We show that the chaotic dynamics of bands at the interfaces of this phase-separated phase results in anomalously slow coarsening.

CPP 21: Poster II

Composites and Functional Polymer Hybrids (1-7), Crystallization, Nucleation and Self-Assembly (8-17), Polymer and Molecular Dynamics, Friction and Rheology (18-22), Modeling and Simulation of Soft Matter (23-38), Glasses and Glass Transition (39-42)

Time: Tuesday 18:00–20:00 Location: Poster E

CPP 21.1 Tue 18:00 Poster E

Tailoring Mesoporous Film Morphologies in Zinc Titanate Oxide via PS-b-PEO Guided Cooperative Self-Assembly — •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 surface-to-volume ratio and pore accessibility of their porous nanostructures. Here, we investigate the morphology evolutions and formation mechanisms of the morphologies of mesoporous zinc titanate oxide films obtained by changing the ratios of two inorganic precursors after calcining hybrid films consisting of organic-inorganic materials. The amphiphilic diblock copolymer self-assembles into micelles in a solvent mixture playing the role of the structure-directing template. The inorganic precursors are loaded in the micellar shell due to hydrogen bonds between poly(ethylene oxide) 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 21.2 Tue 18:00 Poster E

Enhancement of the Protection Performance of Eco-friendly Polymers and Nanoparticles/Polymers Coated Copper Artifact in Synthesized Marine Environments — •Mai Diab[1] and Wafaa Soliman[2] — [1]National Museum of Egyptian Civilization, Cairo, Egypt — [2]National Institute of Laser enhancement Science, Giza, Egypt

Protective coatings based on eco-friendly polymers synthesized from renewable sources (chitosan or glycerol/chitosan polymer) have been prepared for copper artifacts protection from marine corrosion. In addition, the coating efficiency has been improved by adding a protective metal coating for copper as a corrosion inhibitor compound (ZnNi-nanoparticles) to the formulations. An accelerating corrosion test on coated copper substrates was performed to optimize the minimum amount of the inhibitor compound. Dipcoating technique was used to coat the copper specimen's surfaces. Chitosan coating was damaged when it was accelerated under marine corrosive conditions. To solve this problem, ZnNi nanoparticles were added to a chitosan-based solution. It was noticed that the significant addition of ZnNi improved the coating properties. The structural features of the coatings were evaluated by Raman spectroscopy. The surface hydrophobicity was investigated by contact angle measurements. The surface morphology changes of control and coated specimens prior to and after marine aging were evaluated by AFM and SEM. The results show that the 0.2 wt% ZnNi nanoparticles enhanced the efficiency, the mechanical hardness, and the roughness of the specimens.

CPP 21.3 Tue 18:00 Poster E

Engineering a Dual In-Situ Strategy to Incorporate Organotitanium Nanosheets into Polyethylene Terephthalate for High-Performance Outdoor UV Fabric Shelters — •Hailong Yu, Jia Chen, Xiang Fei, Bin Sun, and Meifang Zhu — State Key Laboratory for Modification of Chemical Fibers and Polymer Materials, College of Materials Science and Engineering, Donghua University, 201620, Shanghai, China

In this study, we employed a dual in-situ approach to integrate organotitanium nanosheets into Polyethylene Terephthalate (PET), aiming to explore their applications in high-performance outdoor UV fabric shelters. Characterization techniques, including SEM, XRD, GPC, TGA, DSC, dynamic oscillatory rheology, and capillary rheometer, were utilized. Notably, the study revealed that the nanosheet structure significantly impacted PET's rheological and crystalline behavior, thereby exerting a profound influence on processing performance. We achieved uniform nanosheet dispersion within PET, enhancing structural integrity. PET/nano-Ti composites displayed outstanding UV resistance, with 80% retained strength after UV exposure, surpassing pure PET (70%). UV-A transmittance was only 2.38%, with UPF exceeding 50. These composites offer a robust choice for UV fabric shelters, including outdoor clothing and tents. This research highlights the profound impact of nanosheet composites on PET's behavior and their critical role in UV resistance, supporting the development of high-performance outdoor materials.

CPP 21.4 Tue 18:00 Poster E

Mechanical Response of Carbon Fiber Reinforced Epoxy Composite Parts Joined with Varying Bonding Techniques for Aerospace Applications — •Furkan Karaboğa[1], Yahya Öz[1], Erdem Yunus[2], and Fatih Göleç[2] — [1]Turkish Aerospace, Ankara, Turkey — [2]Bursa Technical University, Bursa, Turkey

Due to the widespread usage of composite materials in aerospace structures, the significance of composite joining methods has been increased. In this research, the impact of various joining techniques on the strength of composite joints through experimental, numerical and analytical analyses is investigated. The study compares the single lap joint shear strengths of carbon fiber reinforced epoxy composites, which are assembled using fastening with pop rivets and solid rivets, secondary bonding, co-curing and co-bonding methods. Additionally, the influence of adhesive thicknesses (from 0.2 to 0.76 mm) for secondary bonding, adhesive film existance for co-bonding and overlapping distance for co-curing on single lap shear strength is explored. Following the production of samples employing different joining methods, tests were conducted according to ASTM 5868. Furthermore, the interface damage in composites was analyzed by using a scanning electron microscope aiming to understand the damage mechanism. Evaluation of fracture mechanisms associated with bonding methods was performed by inspecting the fracture surface of composite samples. The obtained results were also analyzed numerically using software tools. The highest strength is obtained as approximately 25 MPa which deviates only 3 % from the numerical results.

CPP 21.5 Tue 18:00 Poster E

Improvement of Self Healing Functions of Composites via Microvascular Channels — •Eray Kostur[1], Merve Ozkutlu Demirel[1], and Necdet Geren[2] — [1]Turkish Aeorspace, Ankara, Turkey — [2]Cukurova University, Adana, Turkey

Carbon fiber-reinforced polymer (CFRP) composites having high specific strength and modulus, are highly convenient for aerospace and automotive applications which require light-weight and high strength. However, the usage of CFRP is limited by their low crack resistance and poor off-axis strength causing material damage as a result of static and dynamic effects over its service time. Besides, prediction of the failure due to local damages are not reliable so far. This study aims to provide a composite structure with self-healing features through a novel microvascular channel mechanism while preserving its mechanical properties and as a result, to repair micro-sized cracks that occur in its structure. The effect of different channel configurations on mechanical properties is evaluated with mechanical tests. A self- healing agent was injected into microvascular channels and the reaction was triggered by a catalyst which is distributed into matrix, as the crack propagates through the channels. An enhancement of approximately 25 % is observed in the displacement values.

CPP 21.6 Tue 18:00 Poster E

Biopolymer-Templated Deposition of Hierarchical 3D-Structured Graphene Oxide/Gold Nanoparticle Hybrids for Surface-Enhanced Raman Scattering — •Yingjian Guo[1,2], Jungui Zhou[1], Constantin Harder[1,2], Guangjiu Pan[2], Suo Tu[2], Sarathlal Koyiloth Vayalil[1], Daniel Söderberg[4], Peter Müller-buschbaum[2,3], and Stephan V. Roth[1,4] — [1]Deutsches Elektronen-Synchrotron, Hamburg, Germany — [2]TUM School of Natural Sciences, Chair of Functional Materials, 85748 Garching, Germany — [3]MLZ, 85748 Garching, Germany — [4]KTH Royal Institute of Technology, Stockholm, Sweden

Cellulose has emerged as a promising bio-based substrate capable of synergistically combining with conductive materials for diverse applications including sensors, smart windows, and bioelectronics. Typically, Surface Enhanced Raman Scattering (SERS), an advantageous analytical technique, allows for the rapid detection and structural analysis of chemical compounds through their spectral patterns in nanotechnology. Crucial for SERS is fabricating the substrates with strong and reproducible enhancements of the Raman signal over large areas. Herein, we present a straight-forward approach utilizing the layer-by-layer spray coating method to fabricate films loaded with gold nanoparticles and graphene oxide to serve as SERS substrates. To investigate the fundamental mechanisms of enhanced SERS performance, grazing incidence small-angle X-ray scattering was employed to gain comprehensive insights into the nanostructure. Therefore, our approach provides a reference for facile and scalable production of SERS substrates.

CPP 21.7 Tue 18:00 Poster E

Height Distribution of Microparticles in a Local-Light Driven Diffusioosmotic Flow — •Fabian Rohne — Institut für Physik und Astronomie, Karl-Liebknecht-Str.24-25, 14476 Potsdam-Golm

It has been demonstrated that separation of particles of equal size but different surface energies is possible by combination of local-light driven diffusioosmosis (local-LDDO) and microfluidic technology.[1] However, the local-LDDO causes lateral particle repulsion, which results in long-ranged particle-particle interactions observable by an increased horizontal and vertical distance. Here, we present how the height distribution influences drift motion distribution of microparticles along a pressure driven fluid flow, which depends on particle concentration, applied wavelength and fluid low.

[1] Bekir, M.; Sperling, M.; Vasquez Muñoz, D., Braksch, C.; Böker, A.; Lomadze, N.; Popescu, M. N., Santer, S. Advanced Materials 2023, 35, 2300358.

CPP 21.8 Tue 18:00 Poster E

Mechanism for the formation of millimeter-long solid filaments by spin coating dilute solutions of a crystallizable polymer — •Da Huang[1], Thorsten Hugel[2], and Günter Reiter[1] — [1]Institute of Physics, University of Freiburg, Freiburg, Germany — [2]Institute of Physical Chemistry, Albert-Ludwigs-Universität Freiburg, Germany

We investigated the formation of millimeter-long filaments formed by spin-coating dilute para-xylene solutions of rapidly crystallizable polyethylene chains with a contour length in the micrometer range onto mica substrates at high temperatures. These filaments were radially oriented and accumulated at the periphery of the substrate. Our observations can be explained by the stretching of polymers through the flow field induced by spinning the solution on a solid substrate. The corresponding loss in conformational entropy emphasized attractive interactions between polymers, which resulted in the formation of bundles and their assembly into long filaments. Caused by a Plateau-Rayleigh-type instability of a liquid coating on a solid filament and due to crystallization, these filaments were decorated with various small-scale structures. Still in solution, the resulting filaments experienced a Coriolis force as they were dragged towards the periphery of the sample, causing a deviation of their orientation from the radial direction. Finally, filaments adsorbed on the substrate, the solvent evaporated completely and the resulting variety of crystalline patterns and morphologies were examined by various microscopy techniques.

CPP 21.9 Tue 18:00 Poster E

Structure formation in aqueous amine solutions — •Lena Friedrich[1], Dirk Lützenkirchen-Hecht[2], Michael Paulus[1], Aurélien Perera[3], Martina Požar[4], and Christian Sternemann[1] — [1]Fakultät Physik / DELTA, Technische Universität, 44221 Dortmund, Germany — [2]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, 42097 Wuppertal, Germany — [3]Sorbonne Université, Laboratoire de Physique Théorique de la Matière Condensée (UMR CNRS 7600), F75252, Paris cedex 05, France — [4]University of Split, Faculty of Science, 21000 Split, Croatia

Amines are associating liquids that can form transient supramolecular structures via hydrogen bonding [1]. Adding water can significantly alter the liquids' molecular structure. We studied linear, primary amines mixed with various proportions of water, which we heated and cooled, by X-ray diffraction performed at beamline BL8 of DELTA (TU Dortmund). The structure factor pre-peak shows a peculiar concentration dependence when water is added. It significantly gains intensity with increasing water content and shifts to smaller wave-vector transfers. This effect is even more pronounced the longer the carbon chain of the amine is. With temperature increase the intensity of the prepeak decreases. These observations are interpreted in terms of transient cluster formation using molecular dynamics simulations [2]. We thank the BMBF for funding via DAAD in the scope of the French-German collaboration PROCOPE 2024-2025 (Project-IDs 57704875 and 50951YA). [1] L. Almasy et al., PCCP 21, 9317 (2019); [2] M. Požar and A. Perera, J. Mol. Liquids 227, 210 (2017).

CPP 21.10 Tue 18:00 Poster E

Multistep liquid-crystalline ordering of poly(3-hexylthiophene) films induced by the vacuum interface — •Anton Sinner and Oleksandr Dolynchuk — Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Germany

Crystallization in liquids is often initiated at solid-liquid interfaces, which can result in enhanced nucleation kinetics and crystal orientation. However, the influence of the less specific interface to air or vacuum can be of the same importance for ordering phenomena. Elucidating these processes is especially relevant for films of functional polymers, as the structure orientation induced at interfaces can significantly affect the material properties. Here, the influence of the vacuum interface on the crystallization in films of model semiconducting polymer poly(3-hexylthiophene) (P3HT) is investigated. By using in-situ X-ray reflectivity and grazing-incidence X-ray scattering during crystallization upon cooling from the melt, we show that the ordering of P3HT films starts at the vacuum interface and undergoes multiple sanidic liquid-crystalline state (SLCS) transitions. The same hierarchy of SLCS is observed during melting, largely independent of the film thickness. Furthermore, we show that the vacuum interface induces the SLCS transitions at temperatures higher than that of bulk, which still results in a significant thermal hysteresis between cooling and heating. Our results demonstrate that the SLCS formation in P3HT has both similarities and differences to surface freezing of short alkanes at the vacuum interface, providing new insights into the phenomenon.

CPP 21.11 Tue 18:00 Poster E

Semicrystallinity in vitrimers studied by solid-state NMR — Kay Saalwächter and •Fatemeh Fouladi — Institut für Physik - NMR, Betty-Heimann-Str. 7, Martin-Luther Univeristät Halle-Wittenberg, 06120 Halle, Germany

In this study, we investigate the crystalline nature of vitrimer samples with catalyst-controlled bond dynamics by time-domain NMR. The studied vitrimer samples, synthesized by various catalysts to control bond exchange kinetics, feature covalent adaptable networks (CANs) intricately crosslinked through dynamic covalent bonds. The aim is to explore how vitrimeric exchanges influence crystallinity and identify the maximum attainable crystallinity. Specifically, crystallization kinetics was investigated via low-field 1H NMR. The structural diversity in our sample raises questions about the crystallization of alkyl chains or the potential involvement of ester/thioester groups in crystal formation, which is answered by 13C MAS NMR.

CPP 21.12 Tue 18:00 Poster E

Influence of interfacial interactions on the kinetics, morphology, and crystal orientation of interface-induced polymer crystallization — •Marthinus van Niekerk, Oleksandr Dolynchuk, and Thomas Thurn-Albrecht — Experimental Polymer Physics, Institute of Physics, Martin Luther University Halle-Wittenberg, Germany

Initiation of polymer crystallization at an interface to a solid can strongly affect crystallization kinetics that normally surpass that of homogeneous nucleation in the bulk. While heterogeneous nucleation is an activated process occurring below T_m, the process of prefreezing produces a crystalline layer above T_m, which thickens upon cooling. Both prefreezing and heterogeneous nucleation are dependent on interfacial interactions between a polymer and the underlying substrate. We present a systematic study of the crystallization of a model polymer, poly(ϵ-caprolactone) (PCL), on several substrates to elucidate the effects of interfacial interactions. We employ a system of dewetted PCL droplets on various substrates, allowing identification of individual nucleation events. AFM imaging confirms the existence of isolated droplets. Studies with polarized microscopy show large differences in the crystallization rate of PCL droplets during cooling from the melt on different substrates. X-ray scattering shows anisotropic scattering from PCL droplets, which varies according to the substrate, proving that the substrate induces orientation of crystalline lamellae. Thus, we demonstrate the effects of interfacial interactions on interface-induced polymer crystallization.

CPP 21.13 Tue 18:00 Poster E

Influence of Cooling Rate and Molecular Weight on Crystallization of Thin Films of Poly-(3-hexylthiophene) at the Vacuum Interface — •Alexander J. Much and Oleksandr Dolynchuk — Experimental Polymer Physics, Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany

The electronic properties of organic semiconductors in general and semiconducting polymers in particular depend on the crystal orientation. It was previously shown that the interface to air or vacuum induces edge-on orientation in the model semiconducting polymer poly-(3-hexylthiophene) (P3HT) during crystallization from the melt, competing with bulk crystallization. To better understand the kinetics of this crystallization phenomenon, here we investigate the effect of cooling rate on the crystal orientation formed in P3HT films on glass substrates. Furthermore, since molecular weight M_w is known to affect the crystallinity and degree of order in bulk P3HT, we also investigate whether M_w has any effect on the crystal orientation of P3HT films. Using grazing-incidence wide angle X-ray scattering, we show that an increased cooling rate during crystallization from the melt suppresses the formation of edge-on crystals at the vacuum interface in P3HT, resulting in a more isotropic crystal orientation. Meanwhile, there is little to no difference in crystal orientation in films of P3HT with M_w=15kg/mol and M_w=47kg/mol under otherwise identical experimental conditions. Thus, our results demonstrate that the kinetics of P3HT crystallization at the vacuum interface is significantly slower than in the bulk and is weakly dependent on M_w of P3HT.

CPP 21.14 Tue 18:00 Poster E

Integrated Simulation and Experimental Study on the UV Resistance and Crystallization of PA6/TiO2 Nanocomposites — •Hailong Yu[1,2], Jens-Uwe Sommer[2], Bin Sun[1], and Meifang Zhu[1] — [1]State Key Laboratory for Modification of Chemical Fibers and Polymer Materials, College of Materials Science and Engineering, Donghua University, 201620, Shanghai, China — [2]Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, 01069 Dresden, Germany

Addressing the heightened risk from increased UV radiation due to ozone depletion, our study developed PA6/TiO2 nanocomposite fibers with enhanced UV protection. We integrated surface-modified TiO2 nanoparticles into PA6 fibers using a masterbatch blending technique and performed extensive material characterizations. The study centered on the effects of TiO2, modified with agents 550 and 570, on PA6's crystallization. We observed a raised onset temperature and modified crystallinity, significantly influenced by agent 550's grafting effect on PA6's hydroxyl groups. Simulation studies provided further understanding of the structural changes impacting crystallization kinetics. A key achievement of this work is the fibers' exceptional UV resistance, demonstrated by a UPF surpassing 50, making them highly suitable for outdoor applications where robust UV protection is essential.

CPP 21.15 Tue 18:00 Poster E

Engineering Anisotropic Photoluminescence in Quantum Dot Metasurfaces — •Lavanya Beri[1,2], Olha Aftenieva[2], Swagato Sarkar[2], and Tobias A.F. König[2,3] — [1]Indian Institute of Technology Delhi — [2]Leibniz-Institut für Polymerforschung Dresden e.V. (IPF), Hohe straße 6, 01069 Dresden, Germany — [3]Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, Helmholtzstraße 18, 01069 Dresden, Germany

Quantum dots are high-performance, solution-processed materials with high photoluminescence quantum yield. Due to these exceptional properties, quantum dots can serve as building blocks for metasurfaces and are of broad interest for photonic applications. Here, we propose a metasurface with anisotropic photoluminescence due to its structuring. With the help of the template-assisted self-assembly methods [Advanced Functional Materials, 31(36), 2105054], we arrange highly luminescent quantum dots into the so-called blazed grating with intrinsic geometrical asymmetry. The latter modifies quantum dots' otherwise omnidirectional emission profile [ACS nano, 17(3), 2399-2410], enhancing it along the particular resonant directions. We demonstrate the asymmetry of the periodic structure using angle-resolved Fourier spectroscopy. This approach may pave the way toward unidirectional light propagation and lasing [Advanced Optical Materials, 11(6), 2202226].

CPP 21.16 Tue 18:00 Poster E

Probing pre-crystallization dynamics — •Atmika Bhardwaj[1,2], Jens-Uwe Sommer[1,2], and Marco Werner[1] — [1]Institut Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden, Germany — [2]Institute für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01062 Dresden, Germany

Polymer crystallization is a fundamental process influencing material properties, yet understanding the molecular intricacies preceding crystallization remains a challenge. This research builds on our prior work in generating unsupervised machine-learning labels for amorphous and crystalline phases in polymer crystallization [A. Bhardwaj, J.-U. Sommer and M. Werner, arXiv:2311.00454 (2023)]. Our focus extends to the exploration of the polymer melt, to quantify the latent information contained within its molecular conformations prior to crystallization. Through the analysis of the spatial distribution of molecular fingerprints, we characterize the subtle changes in molecular arrangements that precede the crystalline transition. Our study strives to advance the understanding of polymer crystallization, offering a new perspective for informed material design.

CPP 21.17 Tue 18:00 Poster E

Polymer crystallization in bulk and on substrates: flat histogram Monte Carlo simulation — •Evgeniia Filimonova, Timur Shakirov, and Viktor Ivanov — Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany

We use the stochastic approximation Monte Carlo (SAMC) simulation to study crystallization in melts of short polymes chains in the bulk and under confinement (between two hard walls). SAMC allows to sample configurations uniformly over the whole interval of energies in microcanonical ensemble and analyse the transition between amorphous melt at high energies and homogenous crystal at low energies, with a variety of inhomogeneous partially crystalline configurations inbetween. We have proposed new methods for analysis of local crystal ordering based on bond order parameters calculated for properly averaged particle coordinates, which has allowed us to observe the coexistence of domains with different local crystalline symmetries. In melts confined between two walls, 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. Our aim is to identify physical factors which are responsible for one of two possible scenarios of surface-induced polymer crystallization: heterogeneous nucleation or prefreezing.

CPP 21.18 Tue 18:00 Poster E

Molecular dynamics study on the impact of water distribution on nanoscopic friction in case of monolayer MoS_2 — •Miljan Dašić[1,2] and Igor Stanković[2] — [1]Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo náměstí 2, 166 10, Prague, Czech Republic — [2]Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

We have designed and applied a molecular dynamics (MD) simulation setup for the study of nanoscopic frictional phenomena in case of monolayer MoS_2. Our design represents a typical AFM experiment, comprising an amorphous SiO_2 probe in tribo-contact with a monolayer crystalline MoS_2 plate. Based on experimental conditions, we implemented two clearly distinguishable setups, regarding the water distribution: (1) large quantity of water - SiO_2 probe is fully immersed in water and surrounded by water molecules, and (2) ambient water - water coating is attached to the probe, which is surrounded by lateral vacuum gaps. We determined the force-distance characteristics of a fully-immersed probe at several temperatures, revealing that some water molecules get trapped in the probe-plate gap, with their number decreasing as temperature increases. We obtained well-defined stick-slip friction loops via sliding simulations. Considering the slip regime: fully-immersed probe mainly moves in single-slip regime, while ambient water distribution promotes multiple-slips. Amount of water, and especially its distribution, strongly influence the stick-slip frictional behaviour of the studied tribosystem.

CPP 21.19 Tue 18:00 Poster E

Particles Formation in the Drying of Polymer Solution Droplets — •Mengmeng Wu, Hsiao-Ping Hsu, and Kurt Kremer — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, Mainz 55128, Germany

Due to the unique properties such as large specific surface area, high permeability and low density, porous polymer nano- or micro-spheres are promising for various applications including biomedical, pharmaceutical, tissue engineering and degradable electronic applications. We develop a coarse-grained polymer solution droplet model to study the particle structure's formation of drying polymer solution droplets. By inducing a high degree of polymer entanglement and maintaining below the glass transition temperature, highly porous particles are generated followed by a rapid evaporation of the solvent in a vacuum. For a drying droplet in a vacuum, the temperature experiences a decrease owing to solvent vaporization. Such temperature reduction results in a decrease in polymer solubility during evaporation, consequently impacting the drying dynamics of polymer droplets. Our investigation explores how the cooling of droplets during solvent evaporation influences the final morphology of polymer particles.

CPP 21.20 Tue 18:00 Poster E

Diffusion Dynamics in Glassy Polymer Films through MD Simulations — •Sharon Volpe, Hsiao-Ping Hsu, and Kurt Kremer — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, Mainz 55128, Germany

Case II diffusion presents a unique challenge in materials science and polymer engineering. The slow rearrangement of the polymer chains in the glassy state leads to an anomalous sorption behavior: a sharp front is observed as an interface that moves at a constant velocity between the swollen plasticized region and the unswollen glassy region. Unraveling the microscopic mechanisms of Case II diffusion is fundamental for tailoring materials with precise diffusion properties, with applications ranging from drug delivery to food packaging. This study employs Molecular Dynamics (MD) simulations to investigate Case II diffusion in glassy polymer films. A dedicated explicit solvent model is developed to control and vary the solvent-polymer interactions. Our focus is on exploring diffusion for different solvent qualities, their impact on diffusion profiles and the chain characteristics in the swollen region. In certain conditions, the observed diffusion patterns align with the characteristic behavior of Case II diffusion. The simulations provide insights into the interplay between solvent and glassy polymer films and contribute to the knowledge of molecular diffusion in these materials.

CPP 21.21 Tue 18:00 Poster E

Modeling fracture formation and propagation in cured epoxy resins under mechanical stress — •Bariscan Arican[1], Christian Wick[1], and Ana-Sunčana Smith[1,2] — [1]PULS Group, Institute for Theoretical Physics , IZNF, FAU Erlangen-Nürnberg, 91058 Erlangen — [2]Group of Computational Life Sciences, Division of Phys- ical Chemistry, Ruder Bošković Institute, 10000 Zagreb, Croatia

Epoxy resins, integral in manufacturing, play a crucial role due to their versatility. Understanding fracture mechanisms in these materials is paramount for determining mechanical properties. This study focuses on developing a multiscale simulation framework, integrating molecular dynamics (MD) with quantum mechanics/molecular mechanics (QM/MM), to consecutively assess and break bonds, simulating fracture propagation. MD simulations of straining crosslinked epoxy resin extend until the potential occurrence of fracture-inducing bond breakage, determined by bond elongation and referred to as the classical criteria. Subsequently, QM/MM calculations are performed on a small subsystem excised from the main system, precisely identifying actual fracture events through spin contamination assessment. Reaction site topology is then updated with broken bond information to create or propagate the fracture. Classical criteria triggering QM/MM calculations are optimized, ensuring computational resources focus on relevant fracture events. This work provides valuable insights into epoxy resin fracture behavior, advancing our understanding of these materials at the molecular level.

CPP 21.22 Tue 18:00 Poster E

Effects of plasma treatments and temperature on the triboelectric charging behavior of polymers in stirring and shaking charging processes — •Alina Bachmann — Frankfurt am Main, Hessen, Germany

This study evaluates the triboelectric charging behavior of polymers. Examining the effect of different plasma pretreatments and temperatures, the saturation charging of various multi-component polymer blends was conducted.

Within the experimental procedure, the saturation charge through stirring and shaking charging processes was compared. The charge-to-mass ratio and surface charge density serve as crucial parameters for characterising the treated surfaces.

The results of the study find application in the electro-sorting of plastics based on triboelectricity. Since this phenomenon is not scientifically understood to a full extent, the generated data contributes to a more optimised implementation in the technical field.

CPP 21.23 Tue 18:00 Poster E

Balancing short- and long-range interactions in Machine Learning Force Fields — •Tobias Henkes, Igor Poltavsky, and Alexandre Tkatchenko — Université du Luxembourg

Nowadays, highly accurate and data-efficient Machine Learning (ML) Force Fields (FFs) are an established method in computational chemistry and physics. MLFFs can enable simulations of large, complex systems with quantum chemical accuracy by using predefined molecular descriptors or learned representations. However, even state-of-the-art ML models can struggle with handling long- and short-range interactions equally. They often employ a locality assumption, naturally emphasizing short ranges. To overcome this constraint, we embed a coarse-grained description of the global environment into an accurate local atomic representation. Effectively, the ML model now has a balanced picture of local and global features and uses this to simultaneously reproduce long- and short-range effects. We showcase the proposed methodology in the Gradient Domain Machine Learning (GDML) framework. Herein, we utilize a hierarchical descriptor that includes local and global features with adjustable attention weights. The modified GDML approach shows an improved accuracy compared to the default architecture for extended systems such as solvated molecules and liquid water. Ultimately, the developed embedding approach can aid any MLFF model in striking a balance between short- and long-range interactions.

CPP 21.24 Tue 18:00 Poster E

Spiropyran/Merocyanine Amphiphile in Organic and Aqueous Media — •Olga Guskova — IPF Dresden, Dresden, Germany

This theoretical study delves into the molecular and photophysical characteristics of an amphiphilic compound containing spiropyran in both organic and aqueous environments. In organic solvents, the system exhibits positive photochromism: under UV radiation, the colorless spiropyran transitions to a vibrant merocyanine isomer. Conversely, in aqueous solutions, a negative photochromism is observed:

the orange-red merocyanine form becomes more thermodynamically stable in water, and exposure to UV and visible light results in partial or complete photobleaching. The underlying rationale for this phenomenon is elucidated through density functional theory calculations and classical modeling, including thermodynamic integration. The explanation lies in the molecular properties of merocyanine. Following the ring-opening reaction, this molecule transforms into a zwitterionic form. The presence of three charged groups on the periphery of a flat conjugated backbone promotes the self-assembly of merocyanine molecules in water, leading to the formation of elongated associates with stack-like building blocks. Molecular dynamics simulations of the aqueous solution, with a concentration above the critical micelle concentration, confirm this self-assembly phenomenon. This work is supported by DFG. For more information see: V. Savchenko, N. Lomadze, S. Santer, O. Guskova, Int. J. Mol. Sci. 23 (2022) 11535.

CPP 21.25 Tue 18:00 Poster E

Equilibrium self-dissociation free energy of nanoconfined water from classical simulations — •Kira Fischer, Henrik Stooss, and Alexander Schlaich — SC SimTech, University of Stuttgart

Understanding the electrodynamic properties of water in confinement is essential for the development of efficient, cost-effective and environmentally friendly energy storage solutions, in particular water-only batteries. Experiments have shown that the construction of such batteries is possible, but a comprehensive understanding of all the phenomena involved is still lacking. Ab-initio studies have inconclusively reported that the self-dissociation barrier of water might be affected by nano-confinement, but sampling the right ensemble poses an unsolved challenge in such simulations.

In this study, molecular dynamics simulations, including lambda dynamics, are used to investigate the equilibrium self-dissociation of confined water at the nanoscale. We focus on the ion pairs H_3O^+ and OH^-, which are important contributors to the electrodynamic behavior of water, and try to understand the effects of nano-confinement and interfaces on the electrodynamic properties of water.

CPP 21.26 Tue 18:00 Poster E

Atomistic Simulations of Conjugated Polymers - A Bottom-up approach — •Richard Schömig and Alexander Schlaich — SC Simtech, University of Stuttgart, Germany

Conjugated polymers show remarkable properties due to their semiconducting nature and their swelling behaviour in contact with an electrolyte, making them promising materials for next-generation sensors, artificial muscles, artificial synapses or for neuromorphic computing. Their complex band-structure combined with the fine details of doping requires a careful treatment of the electronic structure problem, making computational access to the mechanic response and the swelling dynamics infeasible. On the other hand, established coarse-graining approaches and classical polymer theory will miss important details that characterize the system's response and dynamics. Here, we develop atomistic simulation approaches for the adsorption, swelling, and transport behaviour by means of molecular dynamics simulations. We benchmark our approach against the experimental mechanic behaviour.

CPP 21.27 Tue 18:00 Poster E

Energy conversion during microphase separation in polyoxyethylene-polyoxybutylene diblock copolymers modeled by self-consistent field theory — •Thore Pohl, Huichen Shu, and Michael Fischlschweiger — Clausthal University of Technology, Clausthal-Zellerfeld, Germany

The microscale phase behavior of polyoxyethylene-polyoxybutylene diblock copolymers is particularly intriguing and has already undergone thorough experimental investigation in the literature. Specifically, insitu small-angle X-ray scattering (SAXS) has been employed to characterize phase transition temperatures and polymorphisms. Through these experiments, four distinct microstructures have been identified: cubic, hexagonal, lamellar, and bicontinuous-cubic. Modeling phase transitions, especially the spatial evolution of phases at a microscopic level, remains incomplete for this particular material system. One approach to modeling the polymorphic phase behavior of block copolymers involves utilizing self-consistent field theory (SCFT). Chemical information of the monads is encoded into a set of continuous sequence descriptor functions defined in the contour space domain. In this study, the three-dimensional microstructure and phase behavior of polyoxyethylene-polyoxybutylene diblock copolymers are computed. The interaction functional to be integrated incorporates one interaction energy parameter that is, herein determined inversely through experimental SAXS measurements. Phase change enthalpies for specific compositions and corresponding microstructures could be modeled using SCFT.

CPP 21.28 Tue 18:00 Poster E

Understanding Cellulose-Hemicellulose interactions by molecular dynamics simulation — •Hanieh Mianehrow[1], Yu Ogawa[2], Jakob Wohlert[3], and Silvia Vignolini[1] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam Science Park, Am Mühlenberg 1, 14476 Potsdam — [2]University Grenoble Alpes, CNRS, CERMAV, 38000 Grenoble, France — [3]Department of Fibre and Polymer Technology, Wallenberg Wood Science Center, KTH Royal Institute of Technology, Teknikringen 56, 100 44 Stockholm, Sweden

Structural coloration in plants, achieved through the arrangement of cellulose microfibrils into helicoidal architectures within the cell wall, is a widespread strategy observed in various plant species. However, the mechanism of such organization is not well-understood. This work focuses on studying interactions between cellulose and hemicelluloses, specifically xylan, using molecular dynamics (MD) simulations. Three model xylan chains with different substitution patterns are created, and the extent of their interactions with the cellulose surface is studied by MD simulation. In addition, the conformation of each xylan chain in the presence of cellulose is also investigated. This helps to understand the effect of the substitution pattern on xylan-cellulose interaction. Results show that the substitution pattern of xylan affects the extent of adhesion between xylan and cellulose and the conformation of xylan on cellulose. This could help explain the origin of structural coloration in some plants.

CPP 21.29 Tue 18:00 Poster E

Many-body potentials and optimized mapping schemes for systematic coarse-graining — •Sayan Dutta[1,2,3], Denis Andrienko[4], and Arash Nikoubashman[1,2,3] — [1]Johannes Gutenberg-Universität Mainz — [2]Leibniz-Institut für Polymerforschung — [3]Technische Universität Dresden — [4]Max-Planck Institut für Polymerforschung Mainz

The field of organic semiconductors is largely influenced by diverse molecular compounds which need efficient computational protocols for pre-screening. To reveal the structure-property relationship between the small molecule chemistry and the materials properties that the condensed systems exhibit (like the glass transition temperature), brute-force atomistic molecular simulations are often intractable due to the large gap in relevant length- and time-scales. To tackle these challenges, multi-scale coarse-grained models are promising approaches, which systematically reduce the number of degrees of freedom and smooth the rugged energetic landscapes. Often, the effective coarse-grained potential is approximated by a pairwise interaction which neglects explicit multibody correlations. However, such multibody contributions can play an important role in inhomogeneous systems, such as thin films or droplets, where the local particle density fluctuates strongly. To address this short-coming, we introduce local density dependent potentials (LDP), which include many body interactions in a mean field way. Our computational framework consists of an accurate coarse-grained model, endowed with LDPs, which is expected to improve the coarse-grained model for inhomogeneous systems.

CPP 21.30 Tue 18:00 Poster E

Cononsolvency consequences at finite polymer concentration — •Martin Melčák and Jan Heyda — University of Chemistry and Technology, Prague Technicka 5, 16628, Prague 6 - Dejvice, Czech Republic

Cononsolvency, a rare situation in polymer physics, when a mixture of two good solvents creates a poor solvent, is experimentally known and at the macroscopic level is well-described process. However, despite intensive theoretical and simulation research, the microscopic origin and driving forces behind this phenomenon remain unclear. In this contribution, we employ coarse-grained molecular dynamics simulations to model the chain-chain interaction and aggregation of many polymer chains in explicit solvent-cosolvent mixtures. We have systematically varied the strength of monomer-cosolvent interactions, which resulted in cosolvent exclusion, enrichment, or even bridging. We have calculated effective interactions between two polymer chains, providing a link from the cosolvent effect on a single polymer chain to finite polymer concentrations, utilizing the statistical-thermodynamic framework of Kirkwood-Buff theory. Finally, the cosolvent effect on the polymer state is summarized in the form of a phase diagram.

CPP 21.31 Tue 18:00 Poster E

oxDNA Molecular Dynamics ecosystem applied to the analysis of "Hairygami". — •Michael Matthies[1], Matthew Sample[2], Hao Liu[2], and Petr Šulc[1,2] — [1]Technische Universität München, Garching bei München, Germany — [2]Arizona State University, Tempe, USA

In the rapidly evolving field of nucleic acid and nucleic acid-protein hybrid nanostructure design, computational methods play a crucial role. oxDNA is a popular coarse-grained Molecular dynamics model which recently got extended by an extensive ecosystem. We showcase these improvements on the practical case of analyzing the conformational space of several archetypical rectangular DNA origami structures influenced by oligonucleotide extensions (nicknamed "Hairygami")[1]. These extensions, usually used to attach functional elements to the origami structures induce a curvature of the structures in the bulk. We characterize the phenomenon using the oxDNA ecosystem and provide experimental verification.

[1] M. Sample, H. Liu, M. Matthies, P. Šulc, arXiv:2302.09109 , (2023)

CPP 21.32 Tue 18:00 Poster E

Understanding electrolyte transport properties with interfaces under applied forces: Insight from MD-simulations — •Katharina Kintrup[1], Youssef Mabrouk[1,2], Diddo Diddens[1,2], and Andreas Heuer[1] — [1]Institut für Physikalische Chemie, Corrensstraße 28/30, 48149 Münster, Deutschland — [2]Helmholtz-Institut Münster, Corrensstraße 48, 48149 Münster, Deutschland

Transport properties of electrolytes can be conveniently studied via Molecular dynamics (MD) simulations. However, whereas typically MD simulations are performed with periodic boundary conditions (pbc), experimental systems involve fixed electrodes. As a consequence, the conservation of momentum, observed in MD simulations, is violated. Indeed, previous electrophoretic NMR (eNMR) experiments suggest that the conservation of local volume [1] rather than momentum conservation is the mobility determining constraint.

We performed molecular dynamics (MD) simulations for a simplified binary model, imitating ionic liquids. Starting with an equilibrium configuration, we record the respective center-of-mass velocities after application of an electric field for both boundary conditions and for various box sizes. Whereas in the presence of pbc momentum is naturally conserved, we observe a complex oscillatory time dependence of the two velocities with fixed walls. Their ratio approaches a value nearly compatible with local volume conservation, in qualitative agreement with experiment. A physical picture is formulated, based on the emergence of the generation of standing sound waves. [1] J. Phys. Chem. Lett. 2022, 13, 37, 8761-8767

CPP 21.33 Tue 18:00 Poster E

Orientation of dynamically asymmetric diblock copolymers in shear flow — •Niklas Blagojevic and Marcus Müller — Institut für Theoretische Physik, Universität Göttingen

The ability of diblock copolymers to assemble into periodic structures with length scales in the nanometer range offers many applications. For practical applications, it is often desirable that the microstructures have a high degree of order even on large length scales and are oriented in a desired direction. It is possible to order and orient the microstructures by shearing the copolymer melt. However, the details of the orientation mechanism under shear are not fully understood. In experiments, different orientations are found depending on copolymer type and shear amplitude. Lamellae-forming copolymers were in some cases oriented parallel to the shear gradient and in other cases perpendicular. In our simulations, we analyse the effect of a dynamical asymmetry, where one block has slower time scales than the other. We can show that the parallel orientation is preferred for high dynamic asymmetries while the perpendicular is preferred for small asymmetries. To investigate this, we conducted molecular dynamics simulations of a highly coarse-grained polymer melt using dissipative-particle dynamics under shear flow. We controlled the dynamic asymmetry via a friction parameter as well as via so-called slip-springs, which represent entanglements of the polymers. Different settings were used to determine the stable orientation, for example the simulation of a system with differently oriented lamellae under shear or the simulation of a quench from a disordered state under shear.

CPP 21.34 Tue 18:00 Poster E

Modeling Electronic Coupling in Polymeric Radical Batteries — •Souvik Mitra, Diddo Diddens, and Andreas Heuer — Institut für physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster

We examine the electronic coupling in PTMA, a redox-active polymer often used in organic radical batteries (ORBs). Our study reveals the significant influence of both distance and relative orientation of the redox pairs on the electronic coupling, which suggests that the electronic communication between the redox centres heavily depends on both intramolecular properties as well as the complex intermolecular environment in the electrode material. Additionally, our study highlights the limitations of the frontier molecular orbital (FMO) method in this context. Our findings underline the significance of integrating molecular dynamics and advanced electronic structure methods, like complete active space self-consistent field (CASSCF), to provide a holistic understanding of electronic coupling for charge transfer reactions in organic electrodes. In this framework, we will also introduce a regression analysis designed to predict electronic coupling across various conformations of the redox pairs.

[1] 10.26434/chemrxiv-2023-rn9bj

CPP 21.35 Tue 18:00 Poster E

Aggregation of copolymer chains consisting of flexible and semi-flexible segments: A stochastic approximation Monte Carlo simulation — •Julia Martemyanova, Timur Shakirov, Viktor Ivanov, and Wolfgang Paul — Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany

We use flat histogram Monte Carlo simulations based on the stochastic approximation Monte Carlo (SAMC) algorithm to study aggregation behavior of several multi-block copolymer chains consisting of flexible and semi-flexible segments with equal composition. We compare algorithms with the one-dimensional density of states, which depends on the total energy, and with the two-dimensional density of states, which depends on the energy of intramolecular stiffness and on the energy of non-valence interactions. We present data on different non-trivial morphologies of aggregates, including several structures with high orientational ordering of bonds and with microseparation of segments of different types. Our aim is to identify single chain morphologies which are able to aggregate in a shape-persistent fashion. We also want to learn to which degree such aggregation is stable without the presence of specific interactions like, e.g., hydrogen bonding. We acknowledge the financial support from DFG (project PA 473/18-1).

CPP 21.36 Tue 18:00 Poster E

Stabilizing alpha-Helicity of a Polypeptide in Aqueous Urea — •Luis Andre Baptista dos Santos[1], Yani Zhao[1], Kurt Kremer[1], Debashish Mukherji[2], and Robinson Cortes-Huerto[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Quantum Matter Institute, University of British Columbia, Canada

We propose a mechanism for alpha-helix folding of polyalanine in aqueous urea that reconciles experimental and simulation studies. Over 15μs long, all-atom simulations reveal that, upon dehydrating the protein's first solvation shell, a delicate balance between localized urea residue dipole interactions and hydrogen bonds dictates polypeptide solvation properties and structure. Our work clarifies the experimentally observed tendency of these alanine-rich systems to form secondary structures at low and intermediate urea concentrations. Moreover, it is consistent with the commonly accepted hydrogen-bond-induced helix unfolding, dominant at high urea concentrations. These results establish a structure-property relationship highlighting the importance of microscopic dipole-dipole orientations/interactions for the operational understanding of macroscopic protein solvation.

CPP 21.37 Tue 18:00 Poster E

Heat transport across nanometre-sized gaps — •Oscar Mateos, Pablo M. Martinez, Oscar Gutierrez, Guilherme Vilhena, and Juan Carlos Cuevas — Universidad Autonoma de Madrid, Spain

Calorimetry has recently achieved a significant milestone by measuring heat transport through a single-atom junction, positioning us to investigate heat transfer across various distances, from atom-sized contacts to more extensive separations. When metals come into contact, heat is primarily carried by electrons at close proximity, while at greater distances, it is transported by photons in a Planckian or super-Planckian manner. However, when the separation reaches the nanometer scale, a transition from thermal radiation to conduction is expected. Recent experiments have shown that heat flux between gold contacts at sub-10nm distances exceeded conventional theories by several orders of magnitude, challenging our understanding of heat transfer across vacuum gaps.

In this presentation, we propose to provide an atomic-level description of heat transport across sub-10nm gap between two metallic surfaces with conductivity values ranging nW/K on gaps as large as 5nm. The all-atom molecular dynamics simulations not only provide results in quantitative agreement with the aforementioned experiments but also settle a nearly decade long paradox.

CPP 21.38 Tue 18:00 Poster E

Structure Formation of Nanoparticles on a Polymer Brush: Effect of Polymer-Nanoparticle Interaction — •Bhuwan Poudel, Hsiao-Ping Hsu, and Kurt Kremer — Max Planck Institute for Polymer Research, Mainz, Germany

The prospect of composite materials based on a polymer brush and nanoparticles (NPs) depends on the precise spatial arrangement of NPs within the brush. Therefore, understanding the insertion mechanism and controlling the distribution of NPs in the brush is crucial for optimal applications of nanocomposite materials. We here approach this problem by performing extensive molecular dynamics simulations of the brush-NP system. The brush is described by a weakly semiflexible bead-spring model and NPs are considered as hard spheres of diameter seven times larger than a bead size. As the attraction between polymers and NPs is weak, NPs tend to spread and form a monolayer on the brush surface. The thickness of such a layer is about the size of an NP. As the interaction strength is increased beyond a threshold value, NPs start to penetrate into the brush. Our findings indicate that the assembly of NPs in/on a brush can be precisely controlled by tuning the strength of attraction between polymers and NPs.

CPP 21.39 Tue 18:00 Poster E

Microrheology under pressure using XPCS — •Fiona Berner[1,2], Tobias Ecklund[1,2], Louisa Kraft[1,2], Nele Striker[3], Fabian Westermeier[3], Florian Schulz[4], Felix Lehmkueler[3], Werner Steffen[1], and Katrin Amann-Winkel[1,2] — [1]Max Planck Institute for Polymer Research, Germany — [2]Johannes Gutenberg University, Department of Physics, Germany — [3]Deutsches Elektronen-Synchrotron (DESY), Germany — [4]University Hamburg, Germany

Glycerol is a glass-forming liquid with a glass transition temperature around $T_g \approx 180\,\mathrm{K}$ at ambient pressure. The transition strongly depends on parameters such as the heating and cooling rate. We aimed to investigate the pressure dependence of glycerol's glass transition and viscosity via a microrheological approach, a mixture of 80 % glycerol in water. Our group implemented a diamond anvil cell and a cryostat to the P10 Coherence Applications Beamline of Petra III at DESY.

Coherent X-rays from modern storage-ring-based radiation facilities provide unique capabilities to investigate both the structure and molecular-level dynamics of disordered soft matter systems. X-ray photon correlation spectroscopy (XPCS) can determine the dynamics on the timescale of μs to hundreds of s.

We calculated the intensity auto-correlation function g_2 for small scattering vectors $|\vec{q}|$ and determined the relaxation rate for different pressures and temperatures. We observe that the applied pressure slows down the system, leading to a shift toward a higher glass transition temperature.

CPP 21.40 Tue 18:00 Poster E

Microrheology under pressure using XPCS — •Fiona Berner[1,2], Louisa Kraft[1,2], Tobias Ecklund[1,2], Klara Holl[1,2], Nele Striker[3], Fabian Westermeier[3], Florian Schulz[4], Felix Lehmkueler[3], Werner Steffen[1], and Katrin Amann-Winkel[1,2] — [1]Max Planck Institute for Polymer Research, Germany — [2]Johannes Gutenberg University, Department of Physics, Germany — [3]Deutsches Elektronen-Synchrotron (DESY), Germany — [4]University Hamburg, Germany

Glycerol is a glass-forming liquid with a glass transition temperature around $T_g \approx 180\,\mathrm{K}$ at ambient pressure. The transition strongly depends on parameters such as the heating and cooling rate. We aimed to investigate the pressure dependence of the glass transition and viscosity in a mixture of 80 % glycerol in water, via a microrheological approach. Our group implemented a diamond anvil cell and a cryostat to the P10 Coherence Applications Beamline of Petra III at DESY.

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CPP 21.41 Tue 18:00 Poster E

Temperature-dependent Raman spectroscopic characterization of poly(furfuryl alcohol) — Durval Bertoldo Menezes[1], Francesco D'Amico[2], Thomas Sepperer[3], Artur Benisek[4], and •Maurizio Musso[4] — [1]Instituto Federal do Triângulo Mineiro, Campus Uberlândia, 38.400-970 Uberlandia, Minas Gerais, Brazil — [2]Universitat Salzburg / Fachbereich Chemie und Physik der Materialien — [3]Jakob-Haringer-Strasse 2a — [4]University of Salzburg, Department of Chemistry and Physics of Materials, Jakob-Haringer-Strasse 2a, 5020 Salzburg, Austria

Recently we employed FTIR and Resonant Raman spectroscopy to investigate the chemical constitution of the polymer polyfurfuryl alcohol (PFA) synthetizes in different ways, and appearing macroscopically different: the first one being a liquid and viscous commercial sample, the second one, produced following a thermosetting procedure, being a self-prepared solid and rigid sample.

As a continuation, we have performed a set of temperature dependent Raman spectroscopic measurements in order to study the evolution of these Raman spectra during the glass transition in thermosetted PFA, adopting the same spectral analysis previously performed by us to infer about the glass transition of the polymer poly(methyl methacrylate).

Compatible with Differential Scanning Calorimetry (DSC) data, the Raman spectral features of the thermosetted PFA changed with temperature, this spectral evolution being a clear indication of the PFA glass transition.

CPP 21.42 Tue 18:00 Poster E

Properties of stable ensembles of Euclidean random matrices modeling the vibrations in low-temperature glass — •Philipp Baumgärtel, Florian Vogel, and Matthias Fuchs — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Using coupled disordered harmonic oscillators we investigate the vibrational properties of amorphous solids. Earlier findings suggest that this Euclidean random matrix ensemble features low temperature vibrational anomalies of glasses. By exact numerical diagonalization and a finite size study we analyze the spectra of the harmonic oscillators [1]. We observe a low-frequency regime of extended modes leading to a Debye like vibrational density of states. At larger frequencies the density of states shows an excess over the Debye behavior resembling Wigner's semicircle law. We discuss that the corresponding modes follow the statistics known from the Gaussian orthogonal ensemble. We reveal that the sound waves are damped by Rayleigh scattering even though the ERM system is purely harmonic. Additional calculations performed in two spatial dimension suggest that the two dimensional systems behave very similar to the three dimensional ones.

In conclusion, the Euclidean random matrix model captures salient features of the vibrational phenomena in glass at low temperatures.

[1] P. Baumgärtel, F. Vogel and M. Fuchs. arXiv:2309.08028, 2023

CPP 22: Gels, Polymer Networks and Elastomers I

Time: Wednesday 9:30–11:15 Location: H 0106

Invited Talk CPP 22.1 Wed 9:30 H 0106

Production of various hybrid bio-based gel ink made of polymer grafted nanocellulose, suitable for 3D printing application — •Julien R.G. Navarro, Xuehe Jiang, Feras Dalloul, Enguerrand Barba, and Benedikt Mietner — Institute of Wood Science, University Hamburg, Germany

The use of biodegradable and renewable material resources, which can replace petroleum-based products, to produce performant functional materials are one of the greatest challenges for a future sustainable society. Within this philosophy, bio-based polymers such as nanocellulose have attracted considerable attention. However, nanocellulose needs further chemical surface modification to be considered as suitable ink material in specific applications or for being proceed through 3D gel-printing. This talk will focus on the opportunity and the advantages of modifying the CNF surface chemically through the selective grafting and cross-linking of numerous polymers on its surface, with and without the presence of inorganic nanoparticles. The grafting of those specific entities onto the CNF surface not only affect the behavior of the CNF in suspension, but allows also to introduce numerous new properties before being processed through 3D-printing. In this talk, several gel-ink examples with various properties (luminescent, self-healing, anti-microbial) will be presented and their ability to be 3D printed will be shown.

CPP 22.2 Wed 10:00 H 0106

Predicting birefringence patterns and actuation of 3D-printed structures of liquid crystalline elastomers — •Santiago Gomez Melo, Li-Yun Hsu, Clara Vazquez-Matel, Rasmus Schröder, Eva Blasco, Falko Ziebert, and Ulrich Schwarz — Heidelberg University, Heidelberg, Germany

Liquid crystalline elastomers (LCEs) are a promising class of material to achieve autonomous deformation in response to external stimuli. Their actuation stems from the nematic-isotropic transition of a programmed molecular orientation, in which the LCE locally strains differently along the parallel and perpendicular directions. Recently, interest in this system has increased due to the possibility to 3D-print such materials as structures with arbitrary shapes. Here we show that the orientation in the sample can be controlled by positioning PDMS-scaffolds at the boundaries. Because they introduce strong anchoring boundary conditions, they determine the minimal energy solution of the Landau-de Gennes free energy of the LCE. We show both theoretically and experimentally that the use of suitable scaffold geometries allows for the engineering of diverse textures of the director field, which are then imprinted into the LCE by direct laser writing. To demonstrate successful design, we show that the calculated and measured birefringence patterns agree very well with each other. A similar test can be performed for mechanical actuation by temperature changes, which is predicted by modelling the LCE-microdevice as neo-Hookean material with an active deformation contribution.

CPP 22.3 Wed 10:15 H 0106

Insights into Modelling Cellulose Aerogels: A Computational Approach — Jannik Jarms[1], •Nina Borzecka[1], and Ameya Rege[1,2] — [1]Institute of Materials Research, German Aerospace Center, Köln, Germany — [2]School of Computer Science and Mathematics, Keele University, Staffordshire, England

There is an increasing demand for advanced sustainable materials that can be tailored for very specific applications. In this respect, aerogels have attracted considerable attention due to their extraordinarily high porosity, due to which they provide solutions for various applications such as insulation, sorbents, support for catalysts, etc.

The cellulose aerogel structure is formed due to polycondensation of D-glucose molecules. The structure formation is computationally designed with coarse-grained molecular dynamics. The system of beads represents the monomers, that during synthesis form polymer chains, and subsequently, the final gel structure. The system exhibits the Langevin dynamics which mimics the Brownian motion. The interaction of monomers and polymer chains was implemented as an ensemble of structural and polymer interaction model represented with Hooke's law and Lennard-Jones potential respectively.

The developed approach indicates good agreement with the experiments. Obtained computationally microstructures were characterized in terms of pore structure. Combining experimental and numerical research creates an opportunity for deeper understanding the fundamentals of synthesis of these novel, promising materials.

CPP 22.4 Wed 10:30 H 0106

Systematic Organophilization of Montmorillonite: The Impact Thereof on The Characteristics of NBR and SBR Based Nanocomposites and Their Blends — •Hisham Essawy and Salwa El-Sabbagh — National Research Centre, Cairo - Egypt

Different montmorillonites either, completely hydrophilic (Mont-0), amphiphilic (Mont-25, Mont-50, and Mont-75) or completely hydrophobic (Mont-100) were used as reinforcing fillers for styrene butadiene rubber (SBR) and acrylonitrile butadiene rubber (NBR) individually to predict the influence of the different forms on the properties of the rubbers (rheometric characteristics and mechanical properties). The shifts in the glass transition temperatures (Tg) after the clay insertion were determined from dynamic mechanical thermal analysis (DMTA) to investigate the preference and action of each form. In addition, the storage moduli were used as indications to the corresponding mechanical properties of the samples. The influences could be verified after comparing the impacts of aging conditions on the properties of rubber compositions. The obtained data may provide a platform to suggest the mechanism by which these forms can in some cases act as compatibilizers in addition to their reinforcing/plasticizing effect when employed with the physically incompatible NBR/SBR (50/50) blend, which helps to optimize the properties of nanocomposites based on these blends. The proposed mechanism of action showed good correlation with the results of the mechanical properties and x-ray diffraction (XRD) investigations as well.

CPP 22.5 Wed 10:45 H 0106

Surfactants as a tool for tuning the volume phase transition temperature VPTT of microgels — •Yulia Gordievskaya[1], Joachim Jelken[1], Se-Hyeong Jung[2], Nino Lomadze[1], Andrij Pich[2,3], Elena Yu. Kramarenko[4], and Svetlana Santer[1] — [1]University of Potsdam, Potsdam, Germany — [2]RWTH Aachen University, Aachen, Germany — [3]Aachen Maastricht Institute for Biobased Materials (AMIBM), Maastricht University, Geleen, The Netherlands — [4]Moscow, Russia

Microgels are well-known to be highly responsive systems able to undergo volume phase transitions under changes in various environmental conditions. Due to this feature, they are used as nanocontainers, sensors, micropumps, and actuators in microfluidic systems. We showed the light-driven remote control of the volume phase transition temperature VPTT of p(NIPAM-AAc) microgels between 32°C and up to 95°C in the solution of azobenzene containing surfactants[1,2]. To discuss the mechanism of light-triggered VPTT shift we provided the theoretical calculations covering a wide range of surfactant concentrations and solvent quality. The factors determining the VPTT are electrostatic and hydrophobic interactions in the system and the translational entropy of counterions.

[1] Jelken, J., Jung, S. H., Lomadze, N., Gordievskaya, Y. D., Kramarenko, E. Y., Pich, A., & Santer, S. Adv. Funct. Mater., 2022, 32(2), 2107946. [2]. Schimka S., Gordievskaya Y.D., Lomadze N., Lehmann M., von Klitzing R., Rumyantsev A.M., Kramarenko E.Y., Santer, S. J. Chem. Phys., 2017, 147(3), 031101

CPP 22.6 Wed 11:00 H 0106

Magnetic Controllability in Magnetic Nanogels — •Ivan Novikau[1] and Sofia Kantorovich[1,2] — [1]University of Vienna, Vienna, Austria — [2]Ekaterinburg, Russia

Magnetic Nanogels (MNGs) have emerged as versatile soft materials, especially promising for biomedicine due to the bio-compatibility of external magnetic fields. Recent research has focused on incorporating magnetic nanoparticles (MNPs) into nanogels for targeted drug delivery, enhanced uptake by tumor cells, and advancements in medical imaging and therapy.

This study utilizes molecular dynamics (MD) simulations and the Lattice-Boltzmann (LB) scheme to investigate the magnetic controllability of MNGs. Specifically, we explore the effective transfer of MNP torque to the polymer matrix, providing insights into guiding MNGs through the circulatory system.

For the suspensions of MNGs we calculate the magnetic susceptibility, and analyse the influence of an external magnetic field on viscoelastic properties, with a specific focus on the dynamic moduli.

CPP 23: Modeling and Simulation of Soft Matter III

Time: Wednesday 9:30–11:15 Location: H 0107

CPP 23.1 Wed 9:30 H 0107

FAIR Data Management for Soft Matter Simulations using NOMAD — •Joseph F. Rudzinski[1], José M. Pizarro[1], Nathan Daelman[1], Luca M. Ghiringhelli[2], and Silvana Botti[3] — [1]Institut für Physik und IRIS-Adlershof, Humboldt-Universität zu Berlin, Berlin — [2]Department of Materials Science and Engineering, Friedrich-Alexander-Universität, Erlangen-Nürnberg — [3]RC-FEMS and Faculty of Physics, Ruhr University Bochum, Bochum

NOMAD [nomad-lab.eu][1, 2] is an open-source data infrastructure for materials science data. NOMAD already supports an array of computational codes and techniques, with over 60 parsers that automatically extract essential (meta)data from the raw output of standard calculations. Traditionally, the NOMAD repository has focused on contributions from DFT calculations, accumulating over 12.5 million such entries. More recently, this framework has been expanded considerably, now supporting classical molecular dynamics simulations, as well as complex simulation workflows. In this context, a variety of new features have been implemented into NOMAD, including a schema for defining molecular topologies and system hierarchies. In this talk, I will introduce NOMAD in the context of soft matter simulations, demonstrating some basic functionalities and its potential for improving the data management standards within the classical simulation community through its adherence to the FAIR principles (Findability, Accessibility, Interoperability, Reusability).
[1] Scheidgen, M. *et al.*, JOSS **8**, 5388 (2023).
[2] Scheffler, M. *et al.*, Nature **604**, 635-642 (2022).

CPP 23.2 Wed 9:45 H 0107

Symmetry-adapted polarization learning for vibrational spectroscopy — •David Wilkins — Centre for Quantum Materials and Technologies, School of Mathematics and Physics, Queen's University Belfast, United Kingdom

The polarization of a material system is vital in modelling its response to light, and thus in predicting the results of spectroscopic experiments. However, there are several problems in these kinds of calculations: chief among them the requirement for electronic structure theory calculations and the fact that bulk polarizations are only defined modulo the so-called "quantum of polarization".

The solution of the first of these problems using machine-learning methods, some of which I have developed in the past few years, is by now in the mainstream of computational chemistry, but the second problem is still extant: the polarization is not a continuous function of the atomic positions. In this talk, I will compare and contrast two methods for overcoming this problem, based on localized dipole moments or on localized charges.

While the former method performs best for systems in which long-ranged electrostatics are not important, learning local charges is by far the best method when these effects are important (e.g. in electrolyte solutions). I show how both methods, where they are applicable, lead to very high-quality modelling of infrared and sum-frequency generation spectroscopy.

CPP 23.3 Wed 10:00 H 0107

Vibrational Spectroscopy from Machine Learning Molecular Dynamics by Accurately Representing the Atomic Polar Tensor — •Philipp Schienbein — Department of Physics, Imperial College London, London, SW72AZ, United Kingdom — Department of Physics and Astronomy, University College London, London, WC1E 6BT, United Kingdom

Vibrational spectroscopy is a key technique to elucidate microscopic structure and dynamics. Without the aid of theoretical approaches, it is, however, often difficult to understand such spectra at a microscopic level. Ab initio molecular dynamics has repeatedly proved to be suitable for this purpose, but the computational cost can be daunting; in particular when electronic structure methods beyond GGA DFT are required. Here, a new route to calculate accurate IR spectra from machine learning molecular dynamics is presented, utilizing the atomic polar tensor. The latter can be trained a posteriori on existing molecular dynamics simulations using the E(3)-equivariant neural network e3nn and is a most fundamental physical observable. The introduced methodology is therefore general and transferable to a broad range of systems. Besides benchmarking the method against explicit ab initio molecular dynamics, I will also present applications utilizing a atomic polar tensor neural network at the hybrid DFT level. These demonstrate that it has the potential to significantly contribute toward novel physical findings, especially where large-scale molecular dynamics simulations or expensive electronic structure calculations are required.

CPP 23.4 Wed 10:15 H 0107

Efficient construction of high-dimensional neural network potentials for the Strecker synthesis — •Alea Miako Tokita[1,2], Timothée Devergne[3], A Marco Saitta[3], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany — [3]Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Sorbonne Université, Paris, France

High-Dimensional Neural Network Potentials (HDNNPs) provide potential energy surfaces with the accuracy of electronic structure calculations at strongly reduced computational costs. This enables extended molecular dynamics simulations of large systems such as organic molecules in solution. The construction of a HDNNP for such systems is not a trivial task since they have a vast configuration space which needs to be efficiently sampled. An example for such a complex system is the first step of the classic Strecker-cyanohydrin mechanism for glycine synthesis in water from formaldehyde and hydrogen cyanide. Here, we present a systematic construction of a HDNNP for this system as a showcase for molecular chemistry in solution.

CPP 23.5 Wed 10:30 H 0107

Machine learning of an implicit solvent for dynamic Monte Carlo simulations — Ankush Checkervarty[1], Jens-Uwe Sommer[1,2], and •Marco Werner[1] — [1]Institut Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, Germany

We discuss an implicit solvent model based on an artificial neural network (NN) for dynamic Monte Carlo simulations, where the dynamics is implemented only via local particle displacements (elementary motions). The training data was obtained from coarse grained simulations using the bond fluctuation model with explicit solvent [1] for single homopolymers under variation of solvent quality. The NN based implicit solvent model takes into account only the information of the local environment of monomers in order to predict a distribution of possible acceptance rates [2] of an attempted elementary monomer move in the given configuration. We show that NN-based implicit solvent simulations reproduce the coil-globule transition, as well as dynamic properties such as the bond vector autocorrelation in time and mean square displacements of chain monomers as seen in the explicit solvent model. Furthermore, the learned NN parameters were transferable to a system of multiple homopolymers. [1] C. Jentzsch, M. Werner and J.-U. Sommer, JCP **138**, 094902 (2013). [2] A. Checkervarty, J.-U. Sommer and M. Werner, JCP **158**, 124904 (2023).

CPP 23.6 Wed 10:45 H 0107

Long-Range Descriptors in Atomistic Modeling beyond Electrostatics — •Philip Loche, Kevin Kazuki Huguenin-Dumittan, and Michele Ceriotti — Laboratory of Computational Science and Modeling, IMX, École Polytechnique Fédérale de Lausanne, Switzerland

Over the last decade, the use of machine learning based methods for modelling materials and molecules has developed rapidly. A key ingredient in most successful approaches has been the use of locality, also termed "nearsightedness" of electronic models. Local models truncate atomic interactions beyond some cutoff radius which allows the development of fast algorithms scaling linearly with the number of atoms.

What is systematically neglected in these models are any kind of long-range interactions interactions, including electrostatics, dipole-dipole or van der Waals forces, due to the relatively high computational cost involved.

We present a general mathematical framework that is an extension of the long-range equivariant (LODE) descriptor, and can describe all long-range interactions with an inverse power law form. It can be used to predict scalar target properties (energies) but can also be used in models that need to predict gradients of those (forces). We illustrate how this extension leads to significant improvements in both accuracy and computational cost.

CPP 23.7 Wed 11:00 H 0107

Encapsulation Of Pt-based Clusters In ZIF-8: Insights From First Principles Simulations — •poonam p[1], kathrin l. kollmannsberger[3], waldemar kaiser[2], julien warnan[3], roland a. fischer[3], and alessio gagliardi[1] — [1]Chair of Simulation of Nanosystems for Energy Conversion, Technical University of Munich, Garching bei Munich, Germany — [2]Chair of Theory of Functional Energy Materials, Technical University of Munich, Garching bei Munich, Germany — [3]Department of Chemistry, TUM School of Natural Sciences, Technical University of Munich

The reactivity of Pt-based catalysts dramatically depends on their size and detailed atomic structure. Recently, atom-precise nanoparticles have been generated from molecular ligand-stabilized clusters via encapsulation within MOFs. Our work aims to rationalize the underlying encapsulation mechanism of the ligand-stabilized Pt-based clusters using first-principles simulations. Using Density Functional Theory calculations, we determine the interaction of ZIF-8 precursors with the CO ligands of the Pt-clusters and reveal chemically distinct sites of all the considered clusters, which favor the attraction of Zn2+ ions in solution. AIMD simulations of Pt-based clusters in an explicit methanol solvent model shed light on the competition between the attraction of Zn2+ and the Pt-clusters and the desorption of Zn2+ by solvation with methanol molecules, revealing the importance of bridging CO ligands to create a Zn-rich environment around the Pt-cluster and to guarantee the successful encapsulation.

CPP 24: Responsive and Adaptive Systems I

Time: Wednesday 9:30–11:15 Location: H 0110

Invited Talk CPP 24.1 Wed 9:30 H 0110

Thermoresponsive polymers in aqueous environments: insights by atomistic simulations — •Ester Chiessi — Department of Chemical Science and Technologies, University of Rome Tor Vergata, Via della Ricerca Scientifica I, 00133 Rome, Italy

Atomistic molecular dynamics simulations can reproduce the experimentally observed solution behaviour of thermoresponsive polymers in aqueous environments, accessing hydration features, local conformation and dynamics of the macromolecule, as well as solvent properties. This information contributes to clarify the mechanism of the coil-to-globule, C-G, transition and the influence on this process of polymer stereoregularity and presence of cosolvents/cosolutes, as it will be shown for poly(N-isopropylacrylamide), PNIPAM. Then, using PNIPAM as a reference, simulation results on the solution behaviour in water of other amphiphilic polymers will be presented, including a PNIPAM chemical isomer for which the presence of a lower critical solution temperature, LCST, does not imply a C-G transition. The overall picture suggests that the balance between degree of hydrophilicity and conformational aptitudes of the macromolecule determines the occurrence of a thermally-induced coil-to-globule transition and affects the value of the C-G transition temperature in LCST polymer aqueous solutions.

Acknowledgments. The Italian Ministry of University and Research is acknowledged for financial support through the project PRIN 2022PAYLXW Co-MGELS. The CINECA-ISCRA initiative is acknowledged for computing support.

CPP 24.2 Wed 10:00 H 0110

Soft matter thin films under pressure: a morphological investigation under Grazing Incidence Scattering — •Apostolos Vagias[1,2], Theodore Manouras[3,4], Andreas Buchner[1], Philipp Gutfreund[2], Lionel Porcar[2], Andrew Nelson[5], Leonardo Chiappisi[2], David P. Kosbahn[6], Marcell Wolf[1], Laura Guasco[7,8], Maria Vamvakaki[3,4], and Peter Müller-Buschbaum[1,6] — [1]MLZ, TUM, 85748 Garching, Germany — [2]Institut Laue Langevin (ILL), 38000 Grenoble, France — [3]Institute of Electronic Structure and Laser, Foundation for Research and Technology Hellas, 700 13 Heraklion, Greece — [4]Department of Materials Science and Technology, University of Crete, 700 13 Heraklion, Greece — [5]ANSTO, Lucas Heights, NSW 2234, Australia — [6]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [7]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [8]Max Planck Society Outstation at the MLZ, D-85748 Garching, Germany

Using a custom-designed pressure cell, we tune hydrostatic pressure and combine Grazing Incidence Small Angle Neutron Scattering (GISANS) with specular and off-specular reflectivity under pressure (P) to probe morphologies of soft matter layers immersed in heavy water at P = 1 bar and P = 800 bar. Our results reveal nanostructural rearrangements upon P-increase for a mixture of strongly segregated (hydrophilic) PDMAEMA and (hydrophobic) POFPMA homopolymer brushes anchored on Si substrate.

CPP 24.3 Wed 10:15 H 0110

Investigation of the solvent uptake of salt containing PNIPMAM thin films — •Julija Reitenbach[1], Peixi Wang[1], Linus F. Huber[1], Simon A. Wegener[1], Robert Cubitt[2], Dirk Schanzenbach[3], André Laschewsky[3], Christine M. Papadakis[4], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Institut Laue-Langevin, 71 Avenue des Martyrs, CS 20156, 38042 Grenoble Cedex 9, France — [3]Universität Potsdam, Institut für Chemie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm — [4]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany

Stimuli responsive polymers gained a lot of attention in the past decades due to their unique properties. If polymer thin films exhibit a reversible volume change upon exposure to external stimuli such as temperature, light, pH, or solvents, they become promising candidates for applications such as nanoswitches or sensors. Due to short swelling times and strong volume changes upon solvent incorporation poly(N-isopropyl methacrylamide) (PNIPMAM) thin films are of special interest. In this work, the influence of different salts on the responsivenss of PNIPMAM thin films towards different solvent vapor atmospheres is explored. In situ time-of-flight neutron reflectometry measurements are performed to investigate the macroscopic swelling behavior. To gain further insights on a molecular level and to understand the underlying hydration mechanism, additional in situ Fourier-transform infrared spectroscopy measurements are performed.

CPP 24.4 Wed 10:30 H 0110

Vibrational Spectroscopy of Perdeuterated Poly(N-isopropylacrylamide) Solutions and Hydration Changes Across the Demixing-Transition — •Alfons Schulte[1], Nicolas Harms[1], Eric Rende[1], Dharani Mullapudi[1], Alec Nieth[1], Christopher Bennett[1], Dirk Schanzenbach[2], André Laschewsky[2,3], and Christine M. Papadakis[4] — [1]Physics Department, University of Central Florida, Orlando, USA — [2]Universität Potsdam, Institut für Chemie, Potsdam-Golm — [3]Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm — [4]TUM School of Natural Sciences, TU Munich, Garching

We investigate concentrated aqueous solutions of perdeuterated poly(N-isopropylacrylamide) (PNIPAM-d10) employing Raman scattering and infrared absorption spectroscopy. In comparison to PNIPAM the cloud point temperature increases by several degrees in PNIPAM-d10. In the Raman and infrared spectra four C-D bands are discernible due to stretching vibrations of the alkyl groups. These are analogous to the C-H bands in hydrogenated PNIPAM, however they are shifted to lower frequencies by a factor of 1.4 as expected for the isotope effect. With increasing temperature we observe abrupt red-shifts of the peak frequencies of the C-D bands near 36 C at the demixing transition which are attributed to dehydration of the polymer chains at their coil-to-globule transition.

CPP 24.5 Wed 10:45 H 0110

Dynamic Light Scattering for Characterization of PNIPAM Microgels Subjected to Ultrasound — Sebastian Stock, Leila Sahebmohammadi, Regine von Klitzing, and •Amin Rahimzadeh — Soft Matter at Interfaces, Technical University of Darmstadt, Darmstadt, Germany

Dynamic Light Scattering (DLS) is a widely employed technique for characterizing particles and molecules in solutions/dispersions, offering insights into their size, size distribution, and conformational changes. This study leverages DLS to explore the ultrasound-induced Volume Phase Transition (VPT) of poly(N-isopropylacrylamide) (PNIPAM) microgels. By innovatively integrating ultrasound with a conventional DLS system, we conducted experiments to characterize compact silica particles and microgels under ultrasound influence. Essential parameters, including particle size, frequency, and amplitude of particle vibration, were successfully extracted through analysis of the correlation function of the scattered light intensity. Notably, studies involving non-responsive silica particles demonstrated that ultrasound did not compromise size determination, establishing them as suitable reference systems. Our findings reveal the acousto-responsive nature of PNIPAM microgels, showcasing their ability to undergo VPT over the time of actuation. Microgels exposed to ultrasound exhibit comparable swelling/shrinking behavior to that induced by temperature, albeit with markedly accelerated kinetics. The outcomes of this investigation hold promise for diverse industrial and biomedical applications.

CPP 24.6 Wed 11:00 H 0110

Effect of pressure on the micellar structure of PMMA-*b*-PNIPAM in a water/methanol mixture — •Pablo A. Álvarez Herrera[1], Feifei Zheng[1], Peiran Zhang[1], Julija Reitenbach[1], Heinz Amenitsch[2], Peter Müller-Buschbaum[1], Cristiane Henschel[3], André Laschewsky[3], and Christine M. Papadakis[1] — [1]TU Munich, TUM School of Natural Sciences, Garching, Germany — [2]Elettra Sincrotrone, Trieste, Italy — [3]Universität Potsdam, Institut für Chemie, Potsdam-Golm, Germany

In pure water, amphiphilic block copolymers consisting of a permanently hydrophobic poly(methyl methacrylate) (PMMA) and a thermoresponsive poly(*N*-isopropyl acrylamide) (PNIPAM) block form core-shell micelles. At atmospheric pressure, the solubility of the micellar shell can be altered by changing the temperature or by adding a water-miscible co-solvent. Here, we study the effect of pressure on the phase behavior and micellar structure of PMMA$_{21}$-*b*-PNIPAM$_{283}$ in a 90:10 v/v D_2O/CD_3OD mixture in a pressure range between 10 and 250 MPa. Turbidimetry shows that adding methanol to PMMA-*b*-PNIPAM in D_2O shifts the maximum of the coexistence line to a higher pressure and temperature. Small-angle X-ray scattering reveals the temperature- and pressure-dependence of the core size, shell thickness, shell solvation, micellar correlation, and aggregation behavior of PMMA-*b*-PNIPAM in a water-methanol mixture. We find that adding methanol increases the mobility of the chains forming the micellar core. Also, the degree of solvation and the thickness of the micellar shell feature a maximum at a pressure of around 100 MPa.

CPP 25: Molecular Electronics and Excited State Properties II

Time: Wednesday 9:30–11:00 Location: H 0111

CPP 25.1 Wed 9:30 H 0111

Solvent-Induced Isomerization in Stilbene. Possible Solution to a Longstanding Problem. — •J. Luis Perez Lustres[1], Alexander L. Dobryakov[2], Daria Schriever[1], Martin Quick[3], Ilya Ioffe[4], and Sergey A. Kovalenko[3] — [1]Fachbereich Physik, Freie Universität Berlin — [2]Moscow — [3]Institut für Chemie, Humboldt Universität zu Berlin — [4]Moscow

Stilbene isomerization reaction was studied in the gas phase at collisionless conditions and analysed by RRKM theory [1], which however fails to explain acceleration by buffer gas pressure [2]. In solution, RRKM provides no explanation for, a much faster rate and the small effect of excess excitation energy [3]. We revisited the problem with fs transient absorption in solution at λ_{exc} of 325 and 267 nm. The latter results in a molecular temperature of 600 K at time zero. Consistent with gas phase, an average barrier of 1236 cm^{-1} is deduced in nonpolar solvents. λ_{exc}-dependence is explained by complete IVR and vibrational cooling with a rate constant of 10 ps [4]. This is reconciled with RRKM theory by postulating an additional activation by the solvent, which would be dominant in solution.

References

[1] J. S. Baskin *et al*, *J. Phys. Chem.* **1996**, *100*, 11920-11933. [2] A. Meyer *et al*, *J. Phys. Chem. A* **1999**, *103*, 10528- 10539. [3] S. A. Kovalenko, A. L. Dobryakov, *Chem. Phys. Lett.* **2013**, *570*, 56-60. [4] S. A. Kovalenko *et al*, *J. Chem. Phys.* **2001**, *115*, 3256-3273.

CPP 25.2 Wed 9:45 H 0111

Spatial Anisotropy of the Excitonic Coupling in β-Phase Zinc-Phthalocyanine Single Crystals — •Lisa Schraut-May[1], Kilian Strauss[1], Gabriele Tauscher[2], Heinrich Schwoerer[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg — [3]CAE Bayern, 97074 Würzburg

Since the anisotropic molecular packing in crystalline solids significantly influences their optical properties and their spatial dependence, the microscopic interplay between crystallographic structure, excitonic coupling and resulting optical characteristics defines an important research topic in organic opto-electronics [1]. In this context, metal-phthalocyanines (M-Pc) represent model systems, as they show different polymorphs and can be functionalized e.g. by gradual fluorination of their periphery [2]. In the case of ZnPc, the fluorination leads to changes in the unit cell parameters without strongly affecting the optical properties of the individual molecules. Here, we investigate single crystals of β-phase ZnPc by means of temperature dependent micro-photoluminescence (μ-PL). Besides discussing the microscopic coupling mechanisms associated with the temperature dependent structural changes and leading to superradiant PL enhancement in β-phase ZnPc at cryogenic temperatures, polarization dependent emission studies on various crystallographic facets prepared by microtomy of the crystals complete the picture of excitonic coupling along different crystallographic directions. [1] Hestand et al., Chem. Rev. (2018) [2] Rödel et al., J. Phys. Chem. C (2022)

CPP 25.3 Wed 10:00 H 0111

Large Two-Photon Absorption in Open-Shell N-Heteropolycycles — •Gabriel Sauter[1], Audrey Pollien[2], Kathleen Fuchs[3], Antonia Papapostolou[4], Andreas Dreuw[4], Uwe Bunz[3], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, University Heidelberg — [2]ENS Paris-Saclay, Paris-Saclay University, France — [3]Organisch-Chemisches Institut, University Heidelberg — [4]Interdisciplinary Center for Scientific Computing, University Heidelberg, Germany

We present a study on the third-order nonlinear optical (NLO) properties of organic open-shell compounds, focusing on two-photon absorption (TPA).

TPA provides distinct advantages over single-photon absorption, such as high spatial resolution and penetration depth, while minimizing photodamage. Effective design is crucial for achieving molecules with significant TPA properties. Molecules with a push-pull system, large extended π-system, and rigid planar structure have shown potential for high TPA.

Recent synthesis efforts have focused on N-heteropolycyclic derivatives incorporating this design. By employing the Z-scan technique, we can analyze how molecular design influences NLO properties and find pronounced TPA cross sections in the near-infrared region by introducing open-shell character, revealing remarkable values (up to 8400 GM) compared to similar organic compounds.

CPP 25.4 Wed 10:15 H 0111

Third-Order Nonlinear Optical Properties of N-Heteropolycycles — •Audrey Pollien[1,2], Gabriel Sauter[2], Kathleen Fuchs[3], Uwe Bunz[3], and Petra Tegeder[2] — [1]ENS Paris-Saclay, Paris-Saclay University, Gif-Sur-Yvette, France — [2]Physikalisch-Chemisches Institut — [3]Organisch-Chemisches Institut, Heidelberg University, Heidelberg, Germany

Third-order nonlinear optical (NLO) properties are observed in large

π-conjugated organic molecules, characterized by the polarization of the material depending on the intensity of an applied electromagnetic field, giving rise to valuable properties such as two-photon absorption (TPA), self-focusing, or self-defocusing. Materials exhibiting third-order polarizability are essential for various photonics and optoelectronics applications, including bioimaging, three-dimensional microfabrication, optical data storage, optical limiting, and photodynamic therapy.

We show that open-shell N-heteropolycyclic compounds possess remarkable third-order NLO coefficients although they have a relatively small size and a metal-free nature compared to other molecules reported in the literature with such high properties. They are of particular interest due to their potential applications as photoinitiators and as chiral open-shell N-heteropolycycles in photonics. The third-order NLO properties of N-heteropolycyclic compounds are investigated using Z-scan techniques but also absorption, emission and fluorescence anisotropy measurements are performed for characterization.

CPP 25.5 Wed 10:30 H 0111

Uncovering the influence of OLED host properties on donor-acceptor type TADF emission by single molecule spectroscopy — •Björn Ewald[1], Theodor Kaiser[1], and Jens Pflaum[1,2] — [1]Experimental Physics 6, University of Würzburg, 97074 Würzburg — [2]CAE Bayern, 97074 Würzburg

Molecular emitters exhibiting thermally activated delayed fluorescence (TADF) define a promising class of materials for implementation in commercial Organic Light Emitting Diodes (OLEDs). Their successful application requires an understanding and control of the microscopic TADF dynamics by the complementary host material, in particular its polarity and rigidity. However, the distinct local host emitter interactions and their consequences, e.g. on the dihedral conformation or the emerging charge transfer states, are often obscured by averaging and superimposed effects of the molecular ensemble for a given host. Hence, we introduce single molecule spectroscopy as a powerful tool for uncovering the relevant host-emitter interactions at the molecular level. Our studies on the donor-acceptor type emitter TXO-TPA embedded in amorphous PMMA, (semi-)crystalline UGH-3 and polar DPEPO reveal distinct single-photon emission properties, characteristic for the respective host and clearly discernible by antibunching, bunching and intensity histogramms of the correlated photon statistics as well as by the individual spectral emission. Disclosing such fundamental relations on the single molecule level marks an important step towards understanding specific host-emitter interactions and their application in future TADF-based OLED technologies.

CPP 25.6 Wed 10:45 H 0111

Thiophene-based Polymers in Time Resolved Photoelectron Spectroscopy — •Tobias Reiker[1], Marek K. Charyton[2], Kamil Kotwica[2], Zitong Liu[3], Deqing Zhang[3], Nicolas D. Boscher[2], and Helmut Zacharias[1] — [1]Center for Soft Nanoscience, University of Münster, Germany — [2]Materials Research and Technology Department, Luxembourg Institute of Science and Technology, Esch-sur-Alzette, Luxembourg — [3]Institute of Chemistry, Chinese Academy of Science, Beijing, China

Thiophene-based polymers are promising candidates for solar cell, OLED or transistor (OFET) applications. An internal donor (D) - acceptor (A) system is formed by coupling thiophene polymers with pyrrole chains. The charge transport behavior can be tuned by different alkyl side chains since they influence the electronic structure, HOMO and LUMO level positions, and interchain interactions. With diketopyrrolopyrrole - thiophene (TDPP), diketopyrrolopyrrole - quaterthiophene (PDPP4T) and thienyl-diketopyrrolopyrrole-thieno-thiophene (PDPPTTT) we investigated the electronic dynamics of verified high hole-mobility organic semiconductors. We report results of temporally resolved photoemission studies of thiophene polymers on Silicon substrates. Occupied electronic levels were analysed via static UPS. Dynamic 2PPE experiments were performed for the energetic position and dynamics of the unoccupied states. The systems were studied as deposited by spin coating as well as by oCVD with and without sidechains.

CPP 26: Biomaterials and Biopolymers (joint session BP/CPP)

Time: Wednesday 9:30–13:00 Location: H 1028

Invited Talk CPP 26.1 Wed 9:30 H 1028

Production and applications of artificial spider silk fibers and hydrogels — •Anna Rising — Department of Anatomy Physiology and Biochemistry Swedish University of Agricultural Sciences Uppsala 75007, Sweden — Department of Biosciences and Nutrition, Karolinska Institutet, Neo, Huddinge 14183, Sweden

Spider silk, nature's high-performance fiber, represents an attractive material for many different applications. However, production of the spider silk proteins (spidroins) is problematic due to their repetitiveness and propensity to aggregate.

We have developed a E.coli based production method that generates unprecedented amounts of correctly folded and soluble spidroins. A biomimetic spinning method combined with a protein engineering strategy, result in artificial spider silk fibers that match the toughness of native spider silk. The fibers have successfully been used to guide the extension of neurites in cell culture assays.

In addition, we have discovered that the recombinant spidroins rapidly form self-supporting and transparent hydrogels when incubated at 37 °C. The gelation is associated with the formation of nano-sized fibrils, and spidroin fusion proteins form hydrogels with intact functions of the fusion moieties. By varying the protein concentration, the compressive modulus of the hydrogels can be tuned to match that of skeletal muscle, myocardium and cartilage, respectively. In addition, human mesenchymal stem cells are viable after being encapsulated in the gels, and continuous release of biologics can be achieved as exemplified by an encapsulated cell line producing progranulin.

CPP 26.2 Wed 10:00 H 1028

Understanding the molecular determinants of chitin-protein interactions in the arthropod cuticle - a single-molecule approach — •Ayesha Talib[1,2], Yael Politi[2], and Kerstin G. Blank[1,3] — [1]Max Planck Institute of Colloids and Interfaces, Mechano(bio)chemistry, Am Mühlenberg 1, 14476 Potsdam, Germany — [2]Technische Universität Dresden, CMCB, B CUBE, Tatzberg 41, 01307 Dresden, Germany — [3]Johannes Kepler Universität, Institute of Experimental Physics, Altenberger Straße 69, 4040 Linz, Austria

In the cuticle of arthropods, structural proteins and chitin fibers form a composite material with anisotropic mechanical properties. The molecular parameters that define the chitin-protein interaction are largely unknown. To answer the fundamental question of what controls cuticle mechanical properties, a molecular strategy is employed that integrates protein engineering with single-molecule force spectroscopy. Chitin binding domains (CBDs) from the spider Cupiennius salei have been identified and expressed recombinantly to compare the strength of the protein-chitin interaction. For CBD present in all spider tissues, we investigated three overlapping consensus motifs RR-1, RR-2 and CB-4. Pull-down assays and single-molecule force spectroscopy suggest that the RR-1 motif does not bind to chitin, whereas similar binding strength is observed for the RR-2 and CB-4. We observe a fast dissociation rate, suggesting that CBDs facilitate energy dissipation upon deformation. Our ultimate goal is to correlate molecular properties with the mechanical function of the composite and to synthesize artificial analogues with tunable mechanical properties.

CPP 26.3 Wed 10:15 H 1028

Characterizing bursting spider silk coacervates with micropipette aspiration — •Isabell Tunn[1], Grégory Beaune[2], Jennifer Tersteegen[1], Jaakko V.I. Timonen[2], Francoise Brochard-Wyart[3], and Markus B. Linder[1] — [1]Department of Bioproducts and Biosystems, Aalto University, Finland — [2]Department of Applied Physics, Aalto University, Finland — [3]Institute Curie, Université Paris Sciences et Lettres, Sorbonne Université, Laboratoire Physico Chimie Curie, France

Hollow or core-shell coacervates composed of biomolecules have been reported to serve essential intracellular functions. Recently, numerous hollow and core-shell coacervates have been bioengineered in vitro opening new avenues for their application as drug delivery systems or vessels for chemical reactions. However, the relationship between the molecular structure and the biophysical properties of these coacervates remains largely unexplored. Thus, we characterized the biophysical properties of a set of five bioengineered spider silk protein coacervates using micropipette aspiration. Upon aspiration coacervates can burst like vesicles, demonstrating that protein forms a dense layer (shell) on the surface of the coacervate. To analyse the aspiration and bursting of the hollow coacervates we developed a model, which allows to calculate the surface and bulk viscosity and to estimate the thickness and viscosity of the shell. We anticipate that our model will aid in understanding the formation and properties of hollow coacervates and will facilitate their use as drug delivery systems, reaction vessels as well as material building blocks.

CPP 26.4 Wed 10:30 H 1028

Connecting protein architecture to their emergent droplet properties — •Zhouyi He, Jens-Uwe Sommer, and Tyler Harmon — Leibniz-Institut für Polymerforschung, Institut Theorie der Polymer, 01069, Dresden, Germany

Spatial organization is a fundamental characteristic of biological systems. Biomolecular condensates (droplets) is one class of spatial organization. Understanding how these droplets arise from molecular interactions remains a complex challenge. To address this, we focused on a specific model system consisting of two multivalent proteins with folded domains and disordered linkers which co-phase separate into droplets. We employed coarse-grained simulations to investigate how structural modularity impacts the phase diagram and material properties of these droplets. Our study focuses on the material properties: density, viscosity, and network architecture. The introduction of a coiled-coil domain substantially alters the phase behavior and material properties of the resulting droplets. The stiffness of this domain plays an important role in preventing self-loop closure and thus promoting phase separation, which enables a certain degree of orthogonal design across the various material properties we explored. Our research yields insights into the phase behavior of biomolecular condensates and provides guidelines for the modulation of droplet material properties.

CPP 26.5 Wed 10:45 H 1028

Strain-Controlled Critical Slowing Down in the Rheology of Disordered Networks — •Abhinav Sharma[1,2], Jordan Shivers[3], and Fred MacKintosh[3] — [1]Mathematisch-Naturwissenschaftlich-Technische Fakultät, Universität Augsburg, 86159 Augsburg — [2]Leibniz Institute für Polymerforschung, Dresden — [3]Department of Chemical and Biomolecular Engineering, Rice University, Houston, Texas 77005, USA

Networks and dense suspensions frequently reside near a boundary between soft (or fluidlike) and rigid (or solidlike) regimes. Transitions between these regimes can be driven by changes in structure, density, or applied stress or strain. In general, near the onset or loss of rigidity in these systems, dissipation-limiting heterogeneous nonaffine rearrangements dominate the macroscopic viscoelastic response, giving rise to diverging relaxation times and power-law rheology. Here, we describe a simple quantitative relationship between nonaffinity and the excess viscosity. We test this nonaffinity-viscosity relationship computationally and demonstrate its rheological consequences in simulations of strained filament networks and dense suspensions. We also predict critical signatures in the rheology of semiflexible and stiff biopolymer networks near the strain stiffening transition.

CPP 26.6 Wed 11:00 H 1028

Mechanically biomimetic hydrogel suggests fundamental viscoelastic constraints in intracellular mechanics — •Dorian Marx, Bart Eduard Vos, Till Moritz Münker, and Timo Betz — Drittes Physikalisches Institut - Biophysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The currently best fitting model for the viscoelastic mechanical properties of cellular cytoplasm lacks a connection to physical parameters. To establish this connection, we find and utilize a viscoelastic polyacrylamide-based hydrogel with cytoplasm-like mechanical properties. The variation of experimental parameters reveals the connection of their physical interpretations to the mechanical outcome of the measurement. The used viscoelastic hydrogel enables the comparison of different measurement methods spanning length scales of micrometers (optical tweezers) to centimeters (rheometer) and can serve as a calibration material that is neither ideally elastic nor ideally viscous. Furthermore, a detailed analysis of cellular and hydrogel data uncovers striking correlations of model parameters that closely match between the chemically and physically distinct materials. The results motivate further investigations into the theoretical reasons for the correlations and applications in building artifical cells.

15 min. break

CPP 26.7 Wed 11:30 H 1028

Dynamic DNA origami nanopores — •Anna Baptist[1], Ze Yu[2], Sabina Caneva[2], and Amelie Heuer-Jungemann[1] — [1]MPI of Biochemistry, Martinsried, Germany — [2]TU Delft, The Netherlands

Nanopores are nanoscale structures that form channels across membranes and enable the translocation of molecules. Inspired by naturally occurring pore-forming proteins, different types of artificial nanopores have been created. The DNA origami technique allows for the fabrication of DNA nanostructures with precise control over shape and size that can be modified with a variety of functional molecules. Thus, DNA origami provides a platform for the customized design of nanoscale pores with different channel diameters that can be equipped with anchoring molecules for insertion into lipid membranes. Such nanopores have potential applications in single-molecule sensing, sorting of molecules depending on their sizes or for the fabrication of artificial cells. However, most nanopores created so far are static with a fixed pore diameter. Here, we present a large dynamic DNA origami nanopore that can be mechanically and reversibly switched between different conformations via strand displacement, offering three different pore sizes. After their successful insertion into the lipid bilayer, these nanopores form transmembrane channels with varying diameters depending on their conformation and can be used to control the transport of differently sized molecules across the lipid membrane. Such stimuli-responsive, actuatable nanopores are excellent mimics of complex natural occurring pores, while enabling a higher level of control and a more modular and easily adaptable design.

CPP 26.8 Wed 11:45 H 1028

Nanotextured Surfaces Based on DNA — •Irina Martynenko and Tim Liedl — Faculty of Physics, Ludwig-Maximilians-University, 80539 Munich, Germany

A longstanding goal of material scientists is to fabricate functional materials in which nanoscale objects are precisely positioned on macroscale surfaces. This can be achieved by a combination of bottom-up techniques, such as molecular self-assembly of DNA origami, and top-down lithographic methods. Through DNA origami placement (DOP) on lithographically patterned surfaces a variety of nanoscale components such as organic dyes, proteins or nanoparticles, have already been patterned on large-scale arrays [1, 2]. However, any DOP methods developed so far were limited to two-dimensional DNA origami structures and thus resulted in flat patterns and arrays only. Here we extend DOP to the third dimension through positioning of three-dimensional DNA origami onto nanometer-precise patterns over micro- and even millimeter scales [3]. We demonstrate that our method can produce surfaces nanotextured with three-dimensional hybrid DNA-silica structures with controllable heights up to 50 nm and a feature size down to ~ 6 nm. We believe that the presented strategy can be used for the assembly of a wide range of materials from metals and semiconductors to functional biomolecules arranged in virtually any three-dimensional geometry on large-scale substrates. [1] R. Kershner, Nat Nanotechnol (2009) [2] A. Gopinath, et al., Nature (2016) [3] I. Martynenko et al., Nat Nanotechnol (2023)

CPP 26.9 Wed 12:00 H 1028

DNA-Origami Diamond Crystal with photonic bandgap in the UV Range — •Xin Yin[1], Gregor Posnjak[1], Paul Butler[2], Oliver Bienek[2], Mihir Dass[1], Ian Sharp[2], and Tim Liedl[1] — [1]Ludwig-Maximilian-Universität München, Germany — [2]Walter Schottky Institute, Technical University Munich, Germany

Diamond lattice photonic crystals possess a broad complete photonic bandgap, although its manufacturing has proven challenging. [1] We showcase a DNA origami diamond crystal with 170 nm periodicity. [2] DNA origami is a technique that allows the rational design of complex geometries on the nanoscale, [3] which we apply to build tetrapod single units for the crystal. Pristine crystal formation requires careful control of interactions between the monomers. The thus-formed crystal undergoes silicification, via a wet chemistry method, for enhanced mechanical stability, followed by TiO_2 coating via atomic layer deposition (ALD). The latter process is required to increase the refractive index and thus open the photonic bandgap. Optical measurement reveals a reflection band in UV range, with the peak red shifting as the coating thickness increases. These results align well with simulations predicting the structure's photonic properties. [1] R. K. Cersonsky, J. Antonaglia, B. D. Dice, & S. C. Glotzer. Nature communications, 12(1), 2543. [2] G. Posnjak, X. Yin, P. Butler, O. Bienek, M. Dass, I. D. Sharp, & T. Liedl, arXiv preprint arXiv:2310.10884. [3] P. W. Rothemund. Nature, 440(7082), 297-302.

CPP 26.10 Wed 12:15 H 1028

Scaling properties of RNA as a branched polymer — Domen Vaupotič[1], Angelo Rosa[2], Luca Tubiana[3], and •Anže Božič[1] — [1]Jožef Stefan Institute, Ljubljana, Slovenia — [2]SISSA, Trieste, Italy — [3]University of Trento, Trento, Italy

Formation of base pairs between the nucleotides of an RNA sequence gives rise to a complex and often highly branched RNA structure. While numerous studies have demonstrated the functional importance of the high degree of RNA branching, its topology remains largely unexplored. We use the theory of randomly branching polymers to explore the scaling properties of RNAs by mapping their secondary structures onto tree graphs. Focusing on random RNA sequences of varying lengths, we determine the two scaling exponents related to their topology of branching. Our results indicate that ensembles of RNA secondary structures are characterized by annealed random branching and scale similarly to self-avoiding trees in three dimensions. We further show that the obtained scaling exponents are robust upon changes in nucleotide composition, tree topology, and folding energy parameters. Finally, we demonstrate how the scaling exponents can be obtained from the distributions of the related topological quantities of individual RNA molecules with fixed length. In this way, we establish a framework to study the branching properties of RNA and compare them to other known classes of branched polymers. By understanding the scaling properties of RNA structure we aim to improve our understanding of the underlying principles and open up the possibility to design RNA sequences with desired topological properties.

CPP 26.11 Wed 12:30 H 1028

The role of receptor uniformity in multivalent binding — •Xiuyang Xia[1,2], Ge Zhang[3], Massimo Pica Ciamarra[1], Yang Jiao[4], and Ran Ni[1] — [1]Nanyang Technological University, Singapore — [2]Ludwig-Maximilians-Universität München, Munich, Germany — [3]City University of Hong Kong, Hong Kong, China — [4]Arizona State University, Tempe, USA

Multivalency is prevalent in various biological systems and applications due to the superselectivity that arises from the cooperativity of multivalent binding. Traditionally, it was thought that weaker individual binding would improve the selectivity in multivalent targeting. Here using analytical mean field theory and Monte Carlo simulations, we discover that for receptors that are highly uniformly distributed, the highest selectivity occurs at an intermediate binding energy and can be significantly greater than the weak binding limit. This is caused by an exponential relationship between the bound fraction and receptor concentration, which is influenced by both the strength and combinatorial entropy of binding. Our findings not only provide new guidelines for the rational design of biosensors using multivalent nano-particles but also introduce a new perspective in understanding biological processes involving multivalency.

CPP 26.12 Wed 12:45 H 1028

Salt Effects on Caffeine Across Concentration Regimes — Stefan Hervo-Hansen[1,4], Jakub Polák[2], Markéta Tomandlová[2], Joachim Dzubiella[3], •Jan Heyda[2], and Mikael Lund[4] — [1]Chem. Engineering Div., Osaka Uni., Toyonaka, Osaka 560-8531, Japan — [2]Physical Chem. Dpt., UCT Prague, Technická 5, CZ-16628 Praha 6, Czechia — [3]Physikalisches Inst., Albert-Ludwigs Uni. Freiburg, Hermann-Herder-Straße 3, D-79104 Freiburg im Breisgau, Germany — [4]Theoretical Chem. Div., Lund Uni., Lund SE 221 00, Sweden

This theoretical contribution is motivated by the early work of Charles Tanford, which led to the discovery that molecular surface motifs solvation is proportional to the solvent accessible surface area (SASA). Importantly, later studies have shown that the proportionality constant varies with salt *concentration* and *type*. Using multi-scale computer simulations combined with vapor-pressure osmometry on caffeine-salt solutions, we reveal that this SASA description captures a rich set of molecular driving forces in ternary solutions at changing *solute* and *osmolyte* concentrations.

Central to this theoretical work is a new potential energy function that depends on the instantaneous surface area, salt type, and concentration. Used in *e.g.* Monte Carlo simulations, this allows for a highly efficient exploration of many-body interactions and the resulting thermodynamics at elevated solute and salt concentrations.

This protocol opens the path to account for salt effects on the solvation thermodynamics of molecules of all sizes, including the *salting-in* or *salting-out* of aqueous bio(macro)molecules.

CPP 27: Active Matter III (joint session DY/BP/CPP)

Time: Wednesday 9:30–13:00 Location: BH-N 334

Invited Talk CPP 27.1 Wed 9:30 BH-N 334

Emergent chemotaxis in synthetic active matter — •Abhinav Sharma[1,2], Hidde Vuijk[1], Pierluigi Muzzeddu[3], Holger Merlitz[2], and Jens-Uwe Sommer[2] — [1]Universität Augsburg, 86159 Augsburg — [2]Leibniz Institute für Polymerforschung, Dresden — [3]SISSA, Trieste, Italy

Active particles with their characteristic feature of self-propulsion are regarded as the simplest models for motility in living systems. The accumulation of active particles in low activity regions has led to the general belief that chemotaxis requires additional features and at least a minimal ability to process information and to control motion. We show that self-propelled particles display chemotaxis and move into regions of higher activity if the particles perform work on passive objects, or cargo, to which they are bound. The origin of this cooperative chemotaxis is the exploration of the activity gradient by the active particle when bound to a load, resulting in an average excess force on the load in the direction of higher activity. In fact chemotaxis should emerge in all those structures which allow cooperative exploration of the activity landscape. We demonstrate this in simple assemblies of active molecules, which show robust chemotaxis both under static and dynamic activity landscapes.

CPP 27.2 Wed 10:00 BH-N 334

Active particles interacting via phase-separating chemicals — •Dennis Schorn, Aritra K. Mukhopadhyay, and Benno Liebchen — Institut für Physik Kondensierter Materie, Technische Universität Darmstadt, Germany

Synthetic active particles self-propel by catalyzing a certain chemical reaction and moving up or down the resulting concentration gradient. In this talk, we present our study of the collective dynamics of chemotactic active particles which interact via self-produced chemicals that have an intrinsic tendency to phase separate. When the chemical interactions are attractive (chemoattraction), the particles aggregate to form a large cluster. In contrast, chemorepulsive particles exhibit two distinct patterns: a stationary foam-like structure and an oscillating stripe pattern. We explain the origins of these structures through a comprehensive linear stability analysis of our system. Our findings underscore that the intricate interplay between chemical phase separation and particle chemotaxis induces new instabilities, leading to the formation of unique patterns.

CPP 27.3 Wed 10:15 BH-N 334

Towards the cybernetics of active matter — •Alexander Ziepke[1], Ivan Maryshev[1], Igor S. Aranson[2], and Erwin Frey[1,3] — [1]Arnold Sommerfeld Center and CeNS, LMU, Munich, Germany — [2]Dept. Biomed. Eng., Penn State University, University Park, PA, USA — [3]Max Planck School Matter to Life, Munich, Germany

Cybernetics describes the self-organized behavior of collectives of individual units in response to their environment, often taking inspiration from biological processes. Different organisms have developed various communication strategies to control such collective responses. For instance, social amoeba use chemical signaling to form localized aggregates in response to starvation, insects such as ants secrete pheromones for navigation, and bats and birds employ acoustic signals to form cohesive swarms. Our research focuses on how chemical and acoustic communication enables the formation of collective states with cooperative functionality, a targeted specification of the units, and the control of a coordinated response. In particular, we show that acoustic signaling of oscillatory agents leads to the formation of synchronized localized clusters and collectively propagating snake- and larva-like structures with distinct acoustic signatures. By emitting acoustic waves, these emergent structures are able to sense environmental changes, such as approaching reflective objects, and respond with a coordinated change in phenotype. This study provides insights into design principles for unsupervised microrobots, able to form adaptive, multi-functional structures with population-level cognitive capabilities (Ziepke, Maryshev, Aranson, Frey., Nat Commun 13, 6727 (2022)).

CPP 27.4 Wed 10:30 BH-N 334

Active Spaghetti: Collective Organization in Cyanobacteria — •Jan Cammann[1], Mixon K. Faluweki[2,3], Lucas Goehring[2], and Marco G. Mazza[1] — [1]Loughborough University, UK — [2]Nottingham Trent University, UK — [3]Malawi Institute of Technology

Filamentous cyanobacteria can show fascinating examples of nonequilibrium self-organization, which, however, are not well understood from a physical perspective. We investigate the motility and collective organization of colonies of these simple multicellular lifeforms. As their area density increases, linear chains of cells gliding on a substrate show a transition from an isotropic distribution to bundles of filaments arranged in a reticulate pattern. Based on our experimental observations of individual behavior and pairwise interactions, we introduce a nonreciprocal model accounting for the filaments large aspect ratio, fluctuations in curvature, motility, and nematic interactions. This minimal model of active filaments recapitulates the observations, and rationalizes the appearance of a characteristic length scale in the system, based on the Péclet number of the cyanobacteria filaments.

Reference: M. Faluweki, J. Cammann, et al. Phys. Rev. Lett. 131, 158303 (2023)

CPP 27.5 Wed 10:45 BH-N 334

Collective dynamics and pair-distribution function of active Brownian ellipsoids* — Stephan Bröker[1], •Michael te Vrugt[2], and Raphael Wittkowski[1] — [1]Institut für Theoretische Physik, Center for Soft Nanoscience, Universität Münster, 48149 Münster, Germany — [2]DAMTP, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom

While the collective dynamics of spherical active Brownian particles is relatively well understood by now, the much more complex dynamics of nonspherical active particles still raises interesting open questions. Previous work has shown that the dynamics of rod-like or ellipsoidal active particles can differ significantly from that of spherical ones. In this work [1], we obtain the full state diagram of active Brownian ellipsoids depending on the Péclet number and packing density via computer simulations. The system is found to exhibit a rich state behavior that includes cluster formation, local polar order, polar flocks, and disordered states. Moreover, we obtain numerical results and an analytical representation for the pair-distribution function of active ellipsoids. This function provides useful quantitative insights into the collective behavior of active particles with lower symmetry and has potential applications in the development of predictive theoretical models.

[1] S. Bröker, M. te Vrugt, and R. Wittkowski, arXiv:2307.15535 (2023)

*Funded by the Deutsche Forschungsgemeinschaft (DFG) under Project-IDs 525063330 (MtV) and 283183152 (WI 4170/3) (RW).

CPP 27.6 Wed 11:00 BH-N 334

Flow and orientational properties of active nematic liquid crystals under an electric field — •Yutaka Kinoshita and Nariya Uchida — Department of Physics, Tohoku University, Sendai, Japan

Active nematic liquid crystals are materials where each constituent has nematic symmetry and produces dipolar flow along its axis. Examples include microtubule-kinesin suspensions and actomyosin networks. Because of the input of energy into the system, the state is driven out of thermodynamic equilibrium and shows a chaotic flow called active turbulence. The flow patterns are controlled by external field, confinement, and friction. An external field induces reorientation of the active elements and suppresses chaotic flow. Here we numerically simulate the effects of an electric field on the dynamics of two-dimensional active nematics [1].

We found transitions among three states that are characterized by the degree of flow anisotropy: the active turbulence, laning state, and uniformly aligned state. The average flow speed and its anisotropy are maximized in the laning state. We also found localization of vortices and topological defects associated with periodic shifts between active turbulence and laning state, which is similar to experimentally observed oscillations in a friction-controlled system. Our results might lead to a further understanding of the dynamical states of active nematics under an external field.

[1] Y. Kinoshita and N. Uchida, Phys. Rev. E **108**, 014605 (2023)

15 min. break

CPP 27.7 Wed 11:30 BH-N 334

From Active Chiral Particles to the Active Model B + — •Erik Kalz[1], Abhinav Sharma[2,3], and Ralf Metzler[1,4] — [1]University of Potsdam, Germany — [2]University of Augsburg, Germany — [3]Leibniz-Institute for Polymer Research, Dresden, Germany — [4]Asia Pacific Centre for Theoretical Physics, Pohang, Republic of Korea

A first-principles approach for active chiral hard disks is presented, that explicitly accounts for steric interactions on the two-body level. With a handle on the full derivation, we explicitly point out the necessary assumptions to derive the field-theoretical description for Active Chiral Particles. By considering different regimes of the Péclet number, the well-known models in active matter can be obtained through our consideration. Explicitly, we derive the phenomenological Model B. By going to higher orders in the closure scheme, we show that this first-principles approach results in the recently introduced Active Model B +, a natural extension of Model B for active processes. Contrary to systems without chirality and to previous derivations, we find that chirality can change the sign of the characteristic activity parameters. This has profound consequences for the already shown effects in the Active Model B +. Finally, we draw a connection between Active Chiral Particles and Odd Diffusion, a phenomenon that has attracted considerable attention recently, and for which Active Chiral Particles are handled as an exemplary system.

Ref: E. Kalz, A. Sharma, and R. Metzler: *arXiv preprint arXiv:2310.16691*, 2023

CPP 27.8 Wed 11:45 BH-N 334

Phase Behaviour of a Minimal Chiral Active Ising Lattice Model — •Boyi Wang[1,3], Frank Jülicher[1,4,5], and Patrick Pietzonka[2,1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom — [3]Institute of Physics, Chinese Academy of Sciences, Beijing, China — [4]Center for Systems Biology Dresden (CSBD), Dresden, Germany — [5]Cluster of Excellence, Physics of Life, TU Dresden, Dresden, Germany

We introduce chiral activity into a lattice model with Ising interactions, achieved by locally rotating a random selected 2×2 neighbourhood of lattice site each time step only in clockwise direction. Monte Carlo simulations at low temperature reveal a path to condensate formation, marked by the evolution of the droplet's edge into a particular tilted orientation relative to the square lattice. This tilt angle depends on the local rotation direction, thus reflecting the chirality of the model on a macroscopic scale.

Furthermore, we investigate the stability of the chiral tilted angle in the droplet's lattice field. We identify a persistent edge current flowing along the droplet's interface. By an equivalent 1D model, we also quantify this current-angle dependence, allowing us to identify the angles that emerge in the stationary state.

Our findings provide a novel perspective on chiral non-equilibrium systems in a discrete and analytical framework, expanding our understanding of how chiral driving forces influence the formation and interface behaviour of active droplets.

CPP 27.9 Wed 12:00 BH-N 334

Long-range fluctuation-induced forces in chiral active fluids — Hashem Fatemi[1], Hamidreza Khalilian[1], Jalal Sarabadani[1], and •Reza Shaebani[2] — [1]Institute for Research in Fundamental Sciences (IPM), Iran — [2]Department of Theoretical Physics, Saarland University, Germany

We study long-range fluctuation-induced (FI) interactions in chiral active matter systems. We show that the combination of self-rotation and self-propulsion can lead to large FI forces, depending on the elongation of active particles. Such strong forces can contribute to self-organization of chiral active matter into dynamic structures and patterns. We numerically measure the FI forces between intruders immersed in chiral active fluids and find that the influence of chirality depends on the particle elongation in the active bath. For round active objects, the FI force monotonically decreases with increasing chirality since the active bath structure gradually changes from rotating flocks and vortices to localized spinners. Contrarily, for elongated active objects there is an optimal chiral angle at which the magnitude and range of the FI interaction are maximized. We explain how the balance of collisions around the intruders varies with chirality and separation between the intruders.

CPP 27.10 Wed 12:15 BH-N 334

Self-Solidifying Active Droplets Showing Memory-Induced Chirality — •Aritra K. Mukhopadhyay[1], Kai Feng[2], José Carlos Ureña Marcos[1], Ran Niu[2], Qiang Zhao[2], Jinping Qu[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, 64289 Darmstadt, Germany. — [2]Huazhong University of Science and Technology, 430074 Wuhan, China.

Synthetic microswimmers have yet to achieve the autonomy and versatility of their biological counterparts, particularly in terms of energy supply and motion diversity. Here, we introduce an all-aqueous droplet swimmer that shows remarkable autonomy and rich dynamics without any external driving mechanism [1]. Comprising a surface tension-lowering polyelectrolyte mixture, the droplets undergo self-solidification on acidic water surfaces, gradually emitting polyelectrolytes into the surroundings. A spontaneous asymmetry of the emitted polyelectrolyte concentration along the droplet surface induces Marangoni flows, which causes the droplet to self-propel. The slowly diffusing polyelectrolytes form long-lived chemical trails creating memory effects that drive a dynamic transition from linear to chiral motion. This showcases the droplet's ability to navigate its environment in a persistent, directional manner requiring no externally imposed symmetry breaking. Practical applications are highlighted through the droplets' highly efficient uranium removal from wastewater. Our results provide a route to fueling self-propelled agents that can autonomously perform chiral motion and collect toxins.

[1] K. Feng et al., Advanced Science 10, 2300866 (2023).

CPP 27.11 Wed 12:30 BH-N 334

Optimising transport of active magnetic particles with finite internal magnetic anisotropy — Andrey Kuznetsov[1], Ekaterina Novak[2], Vladimir Zverev[2], Tatyana Belyaeva[2], and •Sofia Kantorovich[1] — [1]University of Vienna, Vienna, Austria — [2]Ekaterinburg, Russia

In recent years, we have observed a rapid development in synthesis techniques that opens up new avenues for tailoring magnetic nanoparticles, including their size, shape, and internal anisotropy. The concept of creating magnetically controllable colloids with finely tuneable rheological properties on the nano- or micro-scale has sparked significant experimental and theoretical efforts but remains not fully realised. In this contribution, we employ molecular dynamics computer simulations to investigate the interplay between internal particle magnetic relaxation dynamics and particle self-propulsion. Our findings demonstrate that optimal transport can be achieved by selecting the strength of an applied magnetic field based on the particle's material and size. This, in turn, opens up an avenue for active magnetic particle sorting.

CPP 27.12 Wed 12:45 BH-N 334

The Role of Anisotropy in Pulsating Active Matter — •Luca Casagrande, Alessandro Manacorda, and Etienne Fodor — University of Luxembourg, Department of Physics and Material Science

Contraction waves have been observed in different biological systems where contractile tissues are present. Some examples can be found in embryonic development, cardiac arrhythmogenesis and uterine contraction. Recently, a particle-based model reproducing the spontaneous emergence of contraction waves has been proposed. In this model, a dense system of active particles is considered, where each particle features isotropic repulsion with neighbors, and has an internal drive that periodically changes its size.*However, it is well know that cells in tissues are not isotropic. Therefore, we consider an additional degree of freedom which embodies the ability of particles to change their eccentricity. It enables us to investigate the role of particle anisotropy in pulsating collective dynamics. The resulting dynamics are studied through numerical simulations. Also an analytical hydrodynamics approach is used through coarse-graining methods. We present the full phase diagram that illustrates the stationary regime as a function of the control parameters of the model. Our model elucidates the interplay between nematic order and phase synchronization in pulsating active matter, and it paves the way towards studying how to control the emergence of contractile waves in biological tissues.

CPP 28: Poster III

Organic Electronics and Photovoltaics (1-30), Hybrid and Perovskite Photovoltaics (31-41), Molecular Electronics and Excited State Properties (42-45), Interfaces and Thin Films (46-53), Electrical, Dielectrical and Optical Properties of Thin Films (54-56)

Time: Wednesday 11:30–13:30 Location: Poster C

CPP 28.1 Wed 11:30 Poster C

Revealing the effect of solvent additive selectivity on formation kinetics in printed active layers for organic solar cells — •Jinsheng Zhang[1] and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]TUM, MLZ, 85748 Garching, Germany

Solvent additives have received tremendous attention in organic solar cells as an effective way to optimize morphology and phase separation. However, most research primarily focuses on solvent additives with superior solvation for non-fullerene acceptors (NFA) over polymer donors, such as the 1-chloronaphthalen (1-CN), 1, 8-diiodooctane (1,8-DIO). Few researches are related to solvent additives characterized by better solubility for polymer donors than NFA. Furthermore, the impact of solvent additives is mainly investigated through spin coating rather than slot-die coating, which exhibits distinct kinetics in film formation. Hence, the influence of solvent additive selectivity on the kinetics of active layer formation in the printed active layer remains unknown. In this study, we use PBDB-T-2F as the donor and BTP-4F as the acceptor and introduce two distinct solvent additives*one with superior solubility for PBDB-T-2F compared to BTP-4F, and the other with inferior solubility for PBDB-T-2F. The drying process of the slot-die coated active layers with different solvent additives is studied by in situ UV-vis absorption spectra and in situ grazing incidence wide angle X-Ray scattering (GIWAXS).

CPP 28.2 Wed 11:30 Poster C

Organic Solar Cells for Space Application: Investigation of the Nanostructure and Degradation Effects Due to Mechanical Stress — •Jan Darsow[1], Lukas V. Spanier[1], Christian Gscheidle[2], and Peter Müller-Buschbaum[1,3] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]TUM School of Engineering and Design, Chair of Astronautics, 85748 Garching, Germany — [3]TUM, MLZ, 85748 Garching, Germany

Organic solar cells (OSCs) are emerging as a promising candidate as an energy source for space applications because of their high gravimetric power density and flexible nature. This would save fuel and space in a rocket flight. However, several challenges must be addressed for OSCs to fulfil their potential in space. Following a previous project that deployed OSCs in space on a suborbital rocket, this work aims to further investigate the degradation of OSCs due to the harsh conditions during space flights. Primarily the degradation due to intense mechanical stress will be investigated. OSCs are exposed to extreme accelerations and vibrations during rocket launch and re-entry. This will be simulated with a shaker stress test followed by an investigation of the OSCs changed structural and electronic properties. The examined OSCs are based on a BTP-4F and PTQ-2F bulk heterojunction (BHJ) and are fabricated on glass and flexible PET substrates. Another topic of this work is research on the effects of annealing the BHJ, which leads to a tuning of the absorption spectrum.

CPP 28.3 Wed 11:30 Poster C

Setup for in Operando X-ray Scattering of Thin Film Solar Cells under Dynamic Temperature Variation — •Simon Alexander Wegener[1] and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]MLZ, TUM, 85748 Garching, Germany

Thin film solar cells hold immense promise for space applications due to their lightweight and flexible nature, making them ideal for powering satellites and spacecraft. Understanding their performance under extreme conditions is pivotal for their successful deployment in space missions. This study introduces an experimental setup designed for operando grazing-incidence wide-angle X-ray scattering (GIWAXS) and grazing-incidence small-angle X-ray scattering (GISAXS) measurements on perovskite and organic thin film solar cells. The setup enables rapid temperature changes, simulating a wide range of operational environments. Crucially, the apparatus exposes solar cells to simulated sunlight of changeable intensity, facilitating measurements under realistic light conditions. Furthermore, it allows modulation of complete day-night cycles, adjusting both, light intensity and temperature up to 130 degrees Celsius to replicate dynamic environmental fluctuations. This methodology offers a comprehensive approach for dynamically evaluating thin film solar cells, providing insights into their structural and functional characteristics under diverse environmental conditions.

CPP 28.4 Wed 11:30 Poster C

Controlling spontaneous orientation polarization in exciplex-forming OLEDs — •Albin Cakaj, Lea Kolb, Alexander Hofmann, and Wolfgang Brütting — Experimental Physics IV, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The resulting internal electrical field, due to spontaneous orientation polarization (SOP), affects the charge injection and accumulation behavior of organic light emitting diodes (OLEDs) significantly. While the community has just recently started to understand the formation process and its active control, it is still not completely clear if this effect is advantageous or detrimental in organic semiconductor devices [1]. In our studies, we investigated an exciplex-forming mixture of the polar species TPBi and the nonpolar molecule TCTA regarding their electrical and optical orientation as well as their properties as an emissive layer in OLEDs. By substrate temperature control the film polarization can be tuned over a broad range from 0 to 125 mV/nm, comparable to recent studies for single-molecule films [2]. But despite of the loose exciton binding, the photoluminescence spectra are not affected by changes in the degree of SOP. Investigations on mixed and bilayer devices hint to the conclusion that exciton quenching is almost not apparent in this material combination. This makes the investigated exciplex system possibly a good candidate as a co-host for efficient OLEDs. [1] A. Hofmann et al. Adv. Optical Mater. DOI:10.1002/adom.202101004 (2021) [2] A. Cakaj et al. ACS Appl. Mater. Interfaces, DOI:10.1021/acsami.3c13049 (2023)

CPP 28.5 Wed 11:30 Poster C

Thickness and Temperature-Dependent Charge Carrier Mobility of Non-fullerene Acceptors in Single-Carrier Electron-Only Devices — •Khawla Alkhezaim, Shahidul Alam, and Frédéric Laquai — King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Physical Sciences and Engineering Division (PSE), Applied Physics Program (AP), Thuwal 23955-6900, Saudi Arabia.

The charge carrier mobility of organic semiconductors is crucial for high-efficiency organic solar cells. This study aims to investigate the charge carrier transport properties in disordered non-fullerene acceptors (NFAs), explicitly focusing on ITIC and its derivatives, namely, ITIC-4F and ITIC-4Cl. The charge carrier transport properties were investigated on single-carrier electron-only devices using the field-independent space-charge-limited-current (SCLC) method. To reveal the impact of order/disorder and halogenation, specifically fluorination or chlorination, thickness and temperature-dependent carrier mobilities were studied systematically. Furthermore, thermionic emission and Fowler-Nordheim tunneling models were applied to calculate the barrier heights at the metal/organic interfaces under forward and reverse bias conditions. Finally, different spectroscopic and microscopic techniques were used to further investigate the optical and morphological properties of the organic semiconductors.

CPP 28.6 Wed 11:30 Poster C

Optimization of Slot-Die Printed Organic Solar Cells — •Christoph G. Lindenmeir[1], Manuel A. Reus[1], Simon Wegener[1], Christopher R. Everett[1], Julian E. Heger[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1,3] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Elettra, 34149 Basovizza, Trieste, Italy — [3]TUM, MLZ, 85748 Garching, Germany

In research, organic solar cells (OSCs) have received a lot of attention in recent years because of their low weight, non-toxicity, short energy payback times and high efficiencies. OSCs are also particularly intriguing to the industry because of their easy solution-based manufacturing technique, which allows for thin and flexible solar cells. The OSCs can be manufactured with different deposition technologies such as printing and spin-coating due to the solution-based fabrication process. Slot-die printing is a very promising printing approach because it is fast, causes low waste and is easily upscalable. Here, we optimize the slot-die printing technique of OSCs under ambient and nitrogen conditions and compare their attributes to spin-coated OSCs. The OSCs are compared using measuring techniques such as spectroscopy and real-space imaging in combination with X-ray scattering.

CPP 28.7 Wed 11:30 Poster C

Characterization of Differently Substituted Imidazo[1,5-a](iso)quinoline Thin Films for Applications as OLED Emitters — •Aaron Pieper[1], Thomas Oel[2], Pascal Schweitzer[1], Carina Rössiger[2], Richard Göttlich[2], and Derck Schlettwein[1] — [1]Institut für Angewandte Physik, Justus-Liebig-Universität Gießen — [2]Institut für Organische Chemie, Justus-Liebig-Universität Gießen

Imidazo-[1,5-a]-quinolines and -iso-quinolines are characterized by an emission in the blue range of the visible spectrum. This can be particularly interesting for applications as emitter molecules in OLEDs. We prepared thin films of differently substituted quinolines and isoquinolines by physical vapor deposition in high vacuum. Their growth mode on technically relevant contact phases like poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) and indium tin oxide (ITO) was studied by non-contact atomic force microscopy. Spectroscopic studies of these thin films were conducted to assess their luminescence and absorbance/excitation properties. First steps were taken to incorporate these materials into a simple OLED layer stack based on PEDOT:PSS as a hole injector and bathocuproine (BCP) as an electron transport layer.

CPP 28.8 Wed 11:30 Poster C

Electroluminescence and Charge Transport Barriers in Blue OLED Based on Thin Films of 3 Phenyl-1-(quinoline-2-yl)imidazo[1,5-a]quinoline — •Pascal Schweitzer[1], Carina Rössiger[2], Alper Yilmaz[1], Gustav Nolte[1], Marius Eckert[1], Richard Göttlich[2], and Derck Schlettwein[1] — [1]Institut für Angewandte Physik, Justus-Liebig-Universität Gießen — [2]Institut für Organische Chemie, Justus-Liebig-Universität Gießen

3-Phenyl-1-(quinoline-2-yl)-imidazo-[1,5-a]-quinoline (PhCIC) is a promising organic emitter molecule for the possible application in blue organic light-emitting diodes (OLEDs). We prepared thin films by physical vapor deposition and studied their photoluminescence (PL) and electroluminescence (EL) to evaluate PhCIC as emitter. Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) served as back contact, poly(9-vinylcarbazole) (PVK) as hole injector, and bathocuproine (BCP) as electron injector contacted by Al. Emission by PVK in the same spectral range as that of PhCIC hindered a detailed discussion. This problem was solved by omitting PVK and the measured EL of PhCIC was in good agreement with PL of PhCIC in solution or as a thin film. To identify the contact responsible for the quite high onset voltage of 10-15 V that we found, film growth and electrical contact formation of PhCIC to PEDOT:PSS and BCP were studied *in situ* by Kelvin probe force microscopy (KPFM). We conclude that charge injection barriers significantly contribute to the onset voltage and possible steps to tune the alignment of transport levels will be discussed.

CPP 28.9 Wed 11:30 Poster C

Film Growth and Work Function of 3-Phenyl-1-(quinoline-2-yl)imidazo[1,5-a]quinoline on Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate and Injection Barriers in a Layered System with Bathocuproine — •Gustav Nolte[1], Pascal Schweitzer[1], Carina Rössiger[2], Richard Göttlich[2], and Derck Schlettwein[1] — [1]Institut für Angewandte Physik, Justus-Liebig-Universität Gießen — [2]Institut für Organische Chemie, Justus-Liebig-Universität Gießen

3-Phenyl-1-(quinoline-2-yl)-imidazo-[1,5-a]-quinoline (PhCIC) is an organic semiconductor which could be applicable in organic light emitting diodes (OLEDs) as a blue emitter. To assess the potential of its application we prepared thin films of PhCIC on poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) by physical vapor deposition and investigated film growth and work function *in situ* by means of Kelvin probe force microscopy (KPFM). Similarly, the film growth of bathocuproine (BCP) on PhCIC was studied. On PEDOT:PSS, PhCIC showed a Stranski-Krastanov type film growth, with the formation of an interface dipole in the base layer and a notable difference in work function between base layer and islands. In contrast, BCP showed a rather homogeneous film growth on PhCIC, forming a space charge region. The alignment of energy levels in the layered system was inferred, showing a significant hole injection barrier from PEDOT:PSS to PhCIC and a smaller barrier for the injection of electrons from BCP to PhCIC.

CPP 28.10 Wed 11:30 Poster C

Transient electroluminescence and current studies on TADF-based OLEDs — •Thomas Fleischmann[1], Björn Ewald[1], and Jens Pflaum[1,2] — [1]University of Würzburg, Faculty of Physics and Astronomy, Experimental Physics VI, 97074 Würzburg — [2]CAE Bayern, 97074 Würzburg

The external quantum efficiency of Organic Light Emitting Diodes (OLEDs) is limited by long-living dark triplet states of conventional fluorophores. This restriction can be lifted by an efficient reverse intersystem crossing (RISC) process which converts non-emissive triplet states into emissive singlet states. This process is prominent in thermally activated delayed fluorescence (TADF) emitters, where the singlet-triplet energy splitting is on the order of thermal energy at room temperature. However, the utilization of TADF emitters comes at the expense of a delayed fluorescence at significantly lower decay rates and a high sensitivity of the photodynamics on the local emitter-host interactions. In this contribution, we analyze the transient behavior of TADF-based OLEDs by applying voltage pulses and recording the time-resolved electroluminescence and current. Comparing these time-resolved properties we conclude on capacitive effects in our OLEDs, e.g. induced by the Schottky-barriers at the contact interfaces, and the photodynamics of the molecular emitters.

CPP 28.11 Wed 11:30 Poster C

P-type PbS CQDs ink for solar cells fabricated via slot-die coating. — •Faryal Talib[1], Huaying Zhong[1], and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]TUM, MLZ, 85748 Garching, Germany

PbS CQDs have demonstrated a greater power conversion efficiency (PCE) of over ˜15% as it utilizes the infrared part of the solar spectrum, making them a compelling candidate for solar cell applications. CQD's ink for solar cells using slot-die coating stems from the potential to streamline the fabrication process and enhance the performance of PbS CQD solar cells. Utilizing the ink and slot-die coating can significantly reduce the need for repetitive layer deposition on the substrate, leading to a more scalable and efficient manufacturing process. This approach addresses the issue of material wastage associated with conventional (solid-state ligand exchange) methods. We are focused on electron-blocking layers (EBLs) of P-type PbS with appropriate ligands to optimize the solar cell's efficiency. The selection of suitable EBL materials with high conductivity, transparency, solution processability, and favorable stability presents a challenge for effective utilization in solar cells.

CPP 28.12 Wed 11:30 Poster C

Calculation of inter-molecular transition rates depending on structural parameters with DFTB — •Fabian Teichert[1], Robin Silligmann[1], Florian Günther[2,3], and Angela Thränhardt[1] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Departamento de Física, Instituto de Geociências e Ciências Exatas, Universidade Estadual Paulista "Júlio de Mesquita Filho", Rio Claro, Brazil — [3]Instituto de Física de São Carlos, Universidade de São Paulo (USP), São Carlos, Brazil

We investigate the transition rates of electrons between two organic molecules, expecially concerning thiophene and zinc porphyrine. 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) two zinc porphyrine molecules. 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 28.13 Wed 11:30 Poster C

Light-Triggered Azobenzene-Bithiophene SAM as a Fullerene Trap — Dmitry Ryndyk and •Olga Guskova — IPF Dresden, Dresden, Germany

Optimizing the efficiency of organic photovoltaic devices may involve strategically utilizing well-defined monolayers containing azobenzene-bithiophene (Azo-BT) switches as electrode modifiers or buffer layers. These monolayers span the interface between the inorganic and organic components, allowing precise control over nanoscale morphology at the electrode. As demonstrated previously [1], cis- and trans-Azo-BT switches chemisorbed on the gold (111) surface exhibit varying geometrical, electronic, and charge transport properties. In this study, we investigate cis-, trans-, and mixed Azo-BT monolayers, with a particular focus on "nanotraps" - nanometer-sized nanopores formed in the monolayers - and their potential to capture C60. Our findings reveal that the photoswitchable "closed" and "open" configurations of Azo-BT nanotraps remain stable at room temperature under experimentally relevant surface densities [2]. We calculate the energies of C60 inside the open nanotrap, demonstrating that the minimum is located inside the pore close to the surface, indicating effective C60 capture. This conclusion is further supported by the Nudged Elastic Band method and Born-Oppenheimer MD calculations. All calculations were performed using the CP2K software (cp2k.org) with the PBE functional, Goedecker-Teter-Hutter pseudopotentials, in conjunction with the DFT-D2 method. [1] Savchenko V. et al. Processes 11 (2023) 2625. [2] Viero Y. et al. J. Phys. Chem. C 119 (2015) 21173.

CPP 28.14 Wed 11:30 Poster C

Dipolar doping of organic semiconductors for photovoltaics — •Patrick Bunk, Hongwon Kim, Albin Cakaj, Alexander Hofmann, and Wolfgang Brütting — Experimental Physics IV, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Previous investigations in the field of organic LEDs showed an improvement in device performance through the doping of dipolar materials, which exhibit a buildup of a giant surface potential (GSP)[1]. However, to the best of our knowledge, dipolar doping has not yet been investigated in the context of organic photovoltaics. For this reason, we investigated prototypical small molecular electron acceptor and donor materials doped with 1,3–Bis[2–(4–tert–butylphenyl)–1,3,4–oxadiazo–5–yl]benzene (Oxd–7) in different ratios using Kelvin Probe (KP). Throughout all doped electron acceptor materials, the GSP was completely suppressed. The doped electron donor (29H,31H–phthalocyaninato(2–)–N29,N30,N31,N32)copper(II) (CuPC) showed a partially suppressed GSP. To investigate the different phases of Oxd-7 in the host material, a Kelvin probe force microscope (KPFM) was used. Furthermore, X-ray diffraction (XRD) measurements led to a better understanding of the orientation of the molecules.

[1] Noguchi et al., Adv. Optical Mater. 2022, 10, 2201278, https://doi.org/10.1002/adom.202201278

CPP 28.15 Wed 11:30 Poster C

Versatile Setup for Gas Phase Spectroscopy of Organic Molecules — •Sebastian Kaiser, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden

In order to gain a better insight into the optical properties and the associated electronic structure of organic semiconductors, it is reasonable to complement the often application-oriented investigations on thin films and solutions with further measurements. Spectroscopy of molecules in the gas phase could resolve vibronic substructures and attenuate ambient effects such as polarization also providing ideal reference data for material simulations. In this contribution, we present a new experimental setup for the spectroscopy of organic semiconductors in gas phase that aims at combining simplicity with efficiency and versatile applicability. The setup is evaluated by using Alq3, MADN, NPB, and TBPe. Sealed under vacuum in a glass ampoule, the materials are heated above the vaporization temperature using hot air. The transparent ampoule allows excitation and detection of emission from the molecules in gas phase with relative ease. However, we also find a strong temperature dependence of the emission spectra resulting from material decomposition, especially for NPB. This is accompanied by a visible discoloration of the cooled material after the measurement. As a first approach, the designed experimental setup is promising. Still, to resolve excitonic substructures, further improvements are required, especially concerning temperature control.

CPP 28.16 Wed 11:30 Poster C

Printed n-type PbS Quantum Dot ink towards solar cells — •Mrinalini Chatterjee[1], Huaying Zhong[1], and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair of Functional Materials, 85748 Garching, Germany — [2]TUM, MLZ, 85748 Garching, Germany

Colloidal Quantum dots (CQDs) have received growing attention in the past decades to produce next generation photovoltaic devices. The quantum confinement effect and size tunability of QDs have enabled customization of their electronic properties, leading to prospective increase in photo-conversion efficiency. Moreover, the solution processibility of QDs has facilitated the single step ink deposition, presenting a more efficient alternative to the conventional layer-by-layer spin-coating method. Despite this, a key challenge remains in realizing high quality, stable ink for active layer deposition for upscaling.

This work focuses on transitioning from conventional spin coating to scalable techniques (slot-die coating) for improved control of film morphology and thickness. To overcome challenges associated with the conventional solvent, Butylamine (BTA), we investigate the effect of alternative solvents including Propylene Carbonate (PC) and Formamide (FA) for the CQD ink, thus optimizing its stability. To do so, characterization techniques such as Fourier transform infrared spectroscopy (FTIR), X ray diffraction (XRD) are used for the chemical and structural analysis. Optical and morphological properties are studied by UV-vis spectroscopy, Scanning electron microscopy (SEM) respectively.

CPP 28.17 Wed 11:30 Poster C

Investigation of structural order at the BF-DPB:BPYMPM donor-acceptor interface by scanning tunneling microscopy — •Milena Merkel[1,2], Philipp Wiesener[1,2], Koen Vandewal[3], and Harry Mönig[1,2] — [1]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Strasse 10, Münster 48149, Germany — [2]Center for Nanotechnology (CeNTech), Heisenbergstrasse 11, Münster 48149, Germany — [3]Institute for Materials Research (IMO-IMOMEC), Hasselt University, Wetenschapspark 1, 3590 Diepenbeek, Belgium

The two molecules B2PYMPM and B4PYMPM serve as electron acceptors in both organic light-emitting diodes and organic solar cells. They differ only in the position of the nitrogen atoms in their lateral pyridine rings, which however leads to the formation of intermolecular hydrogen bonds and subsequent molecular stacking only in the case of B4PYMPM [1]. Paired with the electron donor BF-DPB, the increased structural order of the B4PYMPM molecules results in highly efficient free charge carrier generation [2].

To understand the differences in charge carrier dissociation between the two acceptors, we used a combined approach of scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS). Our STM data with intramolecular resolution comparatively provide insights into the nano-scale self-assembly and inherent intermolecular interactions, which are correlated with XPS core level spectra.

[1] Yokoyama et al., Adv. Funct. Mater., 21, 1375-1382 (2011)

[2] Ullbrich et al., Nat. Mater., 18, 459-464 (2019)

CPP 28.18 Wed 11:30 Poster C

Study on morphology formation of sequential deposition printed organic solar cells — •Lixing Li[1] and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]TUM, MLZ, 85748 Garching, Germany

Layer-by-layer (LbL) organic solar cells (OSCs) exhibit advantages over bulk heterojunction (BHJ) structures due to their interleaved network of donor/acceptor materials and a p-i-n device configuration. The emergence of small-molecule non-fullerene materials has extended the lifetime of excitons, thus making LbL OSCs gain more and more attention. However, most research on LbL OSCs focuses on spin-coating preparation, which may not be applicable for future large-scale production. Our study explores the fabrication of LbL OSCs using printing techniques. PM6 and several different non-fullerene materials are utilized as donors and acceptors, respectively. We use in situ GIWAXS, GISAXS, and UV-vis absorption spectroscopy to investigate morphology formation.

CPP 28.19 Wed 11:30 Poster C

OLED fabrication with a self-designed semi-automated vapor deposition system — •Mona Löther, Ahmed Mohamed, Felix Kübert, Johannes Leser, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, Julius-Maximilians-Universität Würzburg (JMU), 97074 Würzburg

A common method for producing organic light-emitting diodes (OLEDs) involves physical vapor deposition (PVD) of organic and metallic layers in ultra-high vacuum. We have devised a production process featuring a self-designed semi-automated PVD system with two chambers of similar structure - one for organic PVD and the other for metal PVD - connected by an airlock. Each chamber includes a substrate carrier, stepper motors, crystal oscillators for measuring layer thicknesses, rotary-linear motion feedthroughs, and magnetic sensors for precise substrate placement. The organic chamber houses six crucibles, including two pairs of co-evaporating crucibles, while the metal chamber houses two metal boats. The production steps are as follows: placing cleaned ITO-coated substrates in the first chamber, adjusting a mask, sequentially evaporating organics, transferring the substrate to the second chamber without exposure to ambient air, adjusting a different mask, and evaporating metals. A Python program coordinates essential operations such as temperature control, automated positioning of the substrates above the crucibles and metal boats, control of the evaporated layer thickness through shutter control, and data assimilation. The setup has been successfully tested in the fabrication of blue OLEDs based on ν-DABNA.

CPP 28.20 Wed 11:30 Poster C

Temperature-dependent characterization of TADF OLEDs — •Felix Kübert, Ahmed Mohamed, Johannes Leser, Mona Löther, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

When injecting charge carriers into the active layer of an OLED, the electrons recombine in S_1 Singlet and T_1 Triplet states at a 1:3 ratio. Third-generation OLEDs, to achieve fluorescence, use the surrounding thermal energy to lift the electrons from the T_1 state up into the S_1 state, where they can then emit fluorescence; so-called Thermally Activated Delayed Fluorescence (TADF). In this study, OLEDs based on ν-DABNA as emitter material will be characterized in a continuous flow optical cryostat in a wide temperature range. For lower temperatures, the thermal energy in the OLEDs is insufficient for the TADF process, resulting in phosphorescence instead of fluorescence. Meanwhile, charge transport by hopping is also temperature-dependent and needs to be considered. Temperature-dependent measurements on OLEDs will therefore shed more light on the TADF process and further the optimization of OLEDs.

CPP 28.21 Wed 11:30 Poster C

Design and fabrication of blue TADF OLEDs based on ν-DABNA emitter — •Ahmed Mohamed, Mona Löther, Felix Kübert, Johannes Leser, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

Fabrication of efficient blue organic light emitting diodes (OLEDs) is the key challenge for OLED displays. The 2nd generation blue Phosphorescence OLEDs (PHOLED) still show low stability and have the requirements of heavy metals. Thermally activated delayed fluorescence (TADF) is considered a promising alternative of the PHOLED due to the 100% internal quantum efficiency. This study includes the design of a blue TADF OLED with the following structure [Glass/ITO/NPD /TCTA /mCP /mCBP:ν-DABNA /TSPO1 /LiF/Al]. The device was fabricated using a self-built semi-automated thermal evaporation machine with 6 sources in the organic chamber and 2 sources in the metal chamber. The thickness and surface roughness of all the organic and metallic layers were characterized using a thickness profilometer (DEKTAK) and atomic force microscope (AFM). The tooling factors of the quartz crystal monitors was calibrated by measuring the actual thickness of each layer separately. OLED efficiency is characterized by measuring the current-voltage-luminance (IVL), the current efficiency (cd/A), and emission spectra.

Long-term stability of OLEDs were investigated. Optimization of layers thickness and surface roughness leads to further improvements on the stability and efficiency of OLEDs.

CPP 28.22 Wed 11:30 Poster C

In-situ tracking the evolution of morphology and optical properties of thin films during spraying and annealing for organic solar cells — •Shuxian Xiong[1,2], Benedikt Sochor[1], Constantin Harder[1,2], 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

Due to the rapid film formation during spraying, typically over tens of seconds, the resultant morphology is a delicate balance between multiple kinetic processes: solvent evaporation, diffusion of the constituents, phase separation, and ordering. The morphology is strongly rate-dependent, and real-time monitoring is necessary to follow the structural evolution with sufficient time resolution so that the properties of the film can be tailored. Based on the ultrasonic spray deposition technique (a scalable large-area deposition technique), using in-situ grazing incidence small/wide-angle x-ray scattering combined with in-situ annealing, this study pioneered the investigation of the morphology formation process from the liquid state to the final dry film under different spraying conditions. An in-depth understanding of the structural evolution during the non-equilibrium process helps to find the suitable processing parameters to produce thin films with well-performed photovoltaic properties in order to establish the relationship between spray processing control and tailored structures and the performance of polymer solar cell devices.

CPP 28.23 Wed 11:30 Poster C

Detecting photogenerated charge carriers and triplet excitons of NFA-based solar-cell-acceptors using spin-sensitive spectroscopy — •Michael Bulgakov[1], Anastasia Kultaeva[1], Shahidul Alam[2], Vladimir Dyakonov[1], and Andreas Sperlich[1] — [1]Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany — [2]King Abdullah University of Science and Technology, Thuwal 23955-6900,Kingdom of Saudi Arabia

Since non-fullerene acceptors (NFAs) have outperformed their fullerene-based counterparts, there has been a concentrated effort in research to further enhance their performance as acceptor materials in organic solar cells. Contrary to fullerenes, where the C60-molecules provide little possibility for variation, NFAs offer a rich playground for adjusting chain lengths, incorporating functional side chains and further modifications on a molecular level. In this study, we examine five novel and promising materials that came out of this variation process. Using Electron Spin Resonance (ESR) and Optically Detected Magnetic Resonance (ODMR) techniques we detect and analyze charge carrier production and triplet-state recombination processes. The insights obtained from this investigation will offer valuable guidance for further optimizing the functionality of NFAs, paving the way to surpass the 20% performance threshold.

CPP 28.24 Wed 11:30 Poster C

Structure prediction of low-dimensional molecular systems — •Alexey Gudovannyy[1], Martin Pfeiffer[2], Julia M. Schäfer[2], Dirk Hildebrandt[2], and Frank Ortmann[1] — [1]School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Heliatek GmbH, 01139, Dresden, Germany

An increasing number of different structural morphologies realized in organic semiconductor devices became a big challenge for the correct computational modelling of such systems. Methods based on crystal structure prediction became a popular and effective tool for predicting observable crystals used in semiconductors. However, this methodology, like most of its available software implementations, only works with homogeneous 3D systems, which makes modelling modified systems difficult. In this situation, the prediction of low-dimensional molecular systems, i.e., the molecular layer, expands our possibilities for the simulation of different interfaces and morphologies and their mixtures. Here we present an efficient and reliable workflow for the structure prediction of molecular layers, based on a multiscale approach for the structural search of the most thermodynamically stable candidates. Also, we implemented and benchmarked different structure sampling methods and determined the most effective ones. Predictions made were applied to the modelling of various semiconductor systems.

CPP 28.25 Wed 11:30 Poster C

Organic photodiodes for biomedical applications at low light intensities — •Rabiul Islam[1], Siddhartha Saggar[1], Michael Mertig[1,2], and Caroline Murawski[1,2] — [1]Kurt-Schwabe-Institut für Mess- und Sensortechnik Meinsberg e.V., Kurt-Schwabe-Str. 4, 04736 Waldheim, Germany — [2]Technische Universität Dresden, Physikalische Chemie, 01062 Dresden, Germany

We designed organic photodiodes (OPDs) for wearable and implantable optical sensors that are implemented, e.g., in pulse monitoring or fluorescence imaging. Currently, biomedical sensing devices mostly rely on stiff and bulky inorganic semiconductor components and often require additional color filters. In contrast, OPDs enable light detection at higher absorption coefficients and with new form factors being ultra-thin and potentially flexible. Designing organic molecules enables inherent color filtering and device fabrication requires comparably low thermal budgets. All these characteristics make OPDs an ideal candidate for biomedical applications. To detect the often weak intensity signals, OPDs need to possess low dark currents and low noise. In this study, we fabricated solution-based OPDs using P3HT donor and PC71BM acceptor to demonstrate OPDs with reduced dark current, high linear dynamic range, and excellent detection of light intensities as low as 2 pW. Our fabricated OPDs can be used for photoplethysmography to detect the human pulse rate from a fingertip under illumination with white light. Our future research now aims at incorporating the OPDs into functional devices for monitoring neuronal activities by reading fluorescent signals.

CPP 28.26 Wed 11:30 Poster C

Aligning molecular backbones in thin films of organic semiconductors by meniscus guided coating methods — •Robin M. Teichgreber[1], Christopher R. McNeill[2], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]Material Science and Engineering, Monash University, 20 Research Way, Clayton, Australia

The performance of organic solar cells depends crucially on the ability of the generated excitons to diffuse to the donor/acceptor interfaces and to be dissociated there [1]. The exciton transport in the material depends strongly on the morphology of the film, including the orientation of the molecules. The orientation of the molecules is particularly important in highly anisotropic materials. While in previous studies [2][3] the focus was placed primarily on the orientation of the molecules relative to the substrate ("face-on" or "edge-on"), less attention was paid to the role of the orientation of the long axis of the molecules. Investigating the influence of molecular orientation on exciton transport requires samples that exhibit a high degree of alignment. We systematically study such samples using meniscus guided blade coating to gain a fundamental understanding of the physical processes that lead to the alignment of the molecular backbones. We employ methods based on optical spectroscopy and X-ray scattering to characterize the films. [1] Blom, P. W. M. et al. (2007). Advanced Materials. 19, 1551-1566 [2] Rand, B. P. et al. (2012). Advanced Functional Materials. 22, 2987-2995 [3] Ran, N. A. et al. (2017). Nature Communication. 8, 79

CPP 28.27 Wed 11:30 Poster C

Analytical drift-diffusion model for steady-state drain currents in organic electro-chemical transistors — •Andres Unigarro[1] and Florian Günther[2] — [1]Institut für Physik, Technische Universität Chemnitz, Germany — [2]Instituto de Geociências e Ciências Exatas, Universidade Estadual Paulista, Rio Claro, Brazil

Among the different devices developed in the field of organic electronics, organic electrochemical transistors (OECTs) have emerged as potential transducers in applications that require the conversion of ion fluxes to electronic current. For the rational optimization and understanding of the fundamentals of OECTs and OECT-based applications, however, it is essential to have theoretical models capable to predict and recreate the experimental data. The existing models used to describe the OECT functions discussed during the past decade mostly originate from Ohm's law, where the ion flux from the electrolyte into the semiconducting layer takes place only due to an electrical field. But ion migration also occurs upon diffusion. In this work we present an approach to model the ion concentration profile under steady-state conditions based on drift-diffusion principles. This allows to formulate an analytical expression of the source-drain current as a function of gate and drain voltages but also of material parameters like the salt concentration. We show that this allows expressing the volumetric capacitance (a parameter that determines the figure of merit for OECTs) as a function of these material parameters. We furthermore present adjustments of experimental data and comparisons to other OECT models.

CPP 28.28 Wed 11:30 Poster C

Illuminating the dark side of triplet states

— •Mohammad Saeed Shadabroo[1], Dieter Neher[2], and Safa Shoaee[1,3] — [1]Optoelectronics of Disordered Semiconductors, Institute of Physics and Astronomy, University of Potsdam, Potsdam-Golm , Germany — [2]Physics and Optoelectronics of Soft Matter, Institute of Physics and Astronomy, University of Potsdam, Potsdam-Golm , Germany — [3]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., 10117 Berlin, Germany

Optimization of the energy levels at the donor*acceptor interface of organic solar cells has driven their efficiencies to above 19%. However, further improvements towards efficiencies comparable with inorganic solar cells remain challenging because of high recombination losses, mediated by the lowest-energy (singlet and triplet) CT states, which empirically limit the open-circuit voltage (VOC). Using o-IDTBR blended with PM6, we achieve 1.16 V, associated with the achievement of remarkably low non-radiative recombination loss of 160 meV, despite the presence of triplets. In employing the present system as a model example, we elucidate the circumstance wherein, if the triplet lifetime surpasses that of the charge-transfer (CT) decay, the dissociation of triplet excitons to the CT state emerges as a feasible occurrence. This, in turn, serves to reduce the occurrence of an additional loss channel emanating from the T1 state. To shed light on these issues, here, an integrated approach that combines photophysics with device physics is employed in order to establish the relationships among non-radiative recombination losses mediated by the lowest states.

CPP 28.29 Wed 11:30 Poster C

Spark Discharge Doping - Unprecedented Aggregation Control in P3HT Solutions, Films and Blends

— •Fabian Eller and Eva M. Herzig — Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

We introduce a novel solution treatment utilizing spark discharges to enable a highly controlled aggregation of poly(3-hexylthiophene) (P3HT) in solution.[1] By choosing appropriate parameters of this current-induced doping treatment we demonstrate the fine tunability of the aggregate fraction and the quality of the polymer backbone order over exceptionally broad ranges.

When films are processed from highly ordered solutions, the high aggregate quality transfers to the films, which enables a strongly increased hole mobility. The aggregation control of the film formation is especially relevant to overcome the aggregation supression in highly miscible blends, e.g. with Y-series non-fullerene acceptors (NFAs).

[1] F. Eller et al, Small. 19, 2207537, 1613-6810 (2023).

CPP 28.30 Wed 11:30 Poster C

A Theoretical Study of the Optoelectronic Properties of WBDT Covalent Organic Frameworks

— •Laura Fuchs and Frank Ortmann — TUM School of Natural Sciences, Department of Chemistry, Lichtenbergstr. 4, 85748 Garching b. München

Covalent-organic frameworks (COFs) are intriguing materials for optoelectronic applications due to their high tunability of electronic and physical properties. One such example is the electron rich 2D imine-linked WBDT, composed of a Wurster-type motif with N,N,N*,N*-tetraphenyl-1,4-phenylenediamine (W) and benzodithiophene dialdehyde (BDT). Using density-functional theory, we investigate the structure, electronic band structure and density of states of the COF. Additionally, we study electronic transitions and optical properties based on its molecular fragments, focusing on the influence of a careful fragment selection.

CPP 28.31 Wed 11:30 Poster C

Influence of Particle Size on the Formation of Solid Solutions Between MAPbI3 and MAPbBr3

— •Tobias Siegert[1], Fatemeh Haddadi Barzoki[2], Markus Griesbach[1], Christopher Greve[3], Ralf Moos[4], Eva M. Herzig[3], Anna Köhler[1], and Helen Grüninger[2,5] — [1]Soft Matter Optoelectronics — [2]Inorganic Chemistry III — [3]Herzig Group - Dynamics and Structure Formation — [4]Department of Functional Materials — [5]Bavarian Center for Battery Technology (BayBatt), all University of Bayreuth, 95447 Bayreuth, Germany

Mixed halide perovskites, e.g., MAPbI3-xBrx, have emerged as promising candidates to be used as wide-bandgap absorbing layers in tandem solar cell applications due to their tunability of bandgap energy. However, pronounced halide migration, which leads to a severe drop in performance, is still hindering a commercialization. To analyze the halide kinetics, we investigate the thermally driven formation of a solid solution, i.e., halide mixing, between MAPbI3 and MAPbBr3 as a function of the morphology of the perovskite powder. Here, the surface to bulk ratio of the parent powder particles is varied by systematically changing particle sizes.

CPP 28.32 Wed 11:30 Poster C

Influence of unipolar charge carrier injection on lead-halide perovskite nanocrystals

— •Roshini Jayabalan[1], Wolfgang Brütting[1], Theresa Hettinger[2], Marcus Scheele[2], and Yutaka Noguchi[3] — [1]Universität Augsburg, 86135 Augsburg, Germany — [2]Universität Tübingen, 72076 Tübingen, Germany — [3]School of Science and Technology, Meiji University, 214-8571 Kanagawa, Japan

The study on lead halide perovskite nanocrystals (LHP NCs), despite their recent existence, has seen a substantial progress in the research community. Similar to their bulk counterpart, their optical and electrical properties extend to the NCs, with additional advantages including band-gap tuning by size and near unity quantum yield, rendering them as potential emitter material in quantum dot light emitting diodes. With their significantly increased surface area, passivation of surface with appropriate ligands is crucial. While advances in stability and optical properties are outstanding, the electrical accessibility of NCs has gained less attention so far. Efficient electroluminescence relies on a thorough comprehension of the injection of charge carriers into the emitting material. Herein this study, we employ a metal-insulator-semiconductor device structure, with charge selective transport layers to ensure unipolar charge injection (electrons/holes) into the NCs. Finally, we have developed a technique, namely, the displacement current measurenent (DCM) using these devices to understand the electronic properties of LHP NCs films in detail. Trapped charges, injection voltage are identified and carrier specific trends with respect to stabilty are determined.

CPP 28.33 Wed 11:30 Poster C

Fabrication and Characterisation of Cesium-Formamidinium Lead Iodide Perovskite Nanocrystal Layers

— •Thomas Baier[1], Guanjiu Pan[1], Altantulga Buyan-Arivjikh[1], Jinsheng Zhang[1], Yanan Li[1], Matthias Schwartzkopf[2], Sarathlal Koyiloth Vayalil[2], 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

Perovskite quantum nanocrystal solar cells are very promising in contributing to the renewable energy mix of the future being used as active layer within solar cells due to the quantum confinement, which occurs at crystals size below the Bohr radius. They provide high power conversion efficiencies, high photoluminescence quantum yield (PLQY), a narrow PL peak, and are stable in comparison to bulk perovskite. Furthermore, the range of usable X halides (I-, Br-, Cl-) and A cations (FA+, MA+, Cs+) enables fine control of the bandgap over the whole visible spectrum of the ABX3 perovskite structure.

Cesium-formamidinium lead iodide perovskite nanocrystal layers have been prepared using different washing processes between several deposition steps, as well as changing the ratio between cesium lead iodide and formamidinium lead iodide perovskite nanocrystals. Therefore different measurement (PL, UV-Vis, microscopy, and SEM) and deposition techniques (spin-coating, and slot-die coating) were used to obtain the optoelectronic properties of the final film.

CPP 28.34 Wed 11:30 Poster C

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], Guangjiu Pan[1], Yusuf Bulut[2], Kristian Reck[3], Thomas Strunskus[3], Franz Faupel[3], Stephan V. Roth[2], 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]Lehrstuhl für Materialverbunde, Institut für Materialwissenschaft, Christian Albrechts-Universität zu Kiel, 24143 Kiel, Germany — [4]TUM, MLZ, 85748 Garching, Germany

It is crucial to suppress the non-radiation recombination in the hole-blocking layer (HBL) and at the interface between the HBL and active layer for performance improvement. We deposited a TiOx thin layer atop the SnO2 layer via sputter deposition at room temperature as an interface modification layer. The structure evolution of TiOx during sputter deposition is investigated via in situ grazing-incidence small-angle X-ray scattering. The HBL, combined with the TiOx interface modification layer, shows a suitable transmittance, smoother surface roughness, and fewer surface defects, thus resulting in 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 28.35 Wed 11:30 Poster C

Enhanced Air Stability of Tin Based Perovskite Solar Cells with Quercetin — •Xiaojing Ci[1] and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]TUM, MLZ, 85748 Garching, Germany

As the most essential alternative materials for eco-friendly perovskite solar cells (PSCs), tin-based perovskites have achieved an efficiency of 14.81 %, which is far less than 25.7 % of lead-based champion devices. The main reason is that it is easy to oxidize Sn2+ to Sn4+ in the presence of oxygen and water due to the low stability of the Sn2+ state. The oxidation of Sn2+ will form vacancies in the perovskite structure, leading to p-type self-doping and introducing additional defect states. These defects can enhance the device's leakage current and charge carrier recombination, limit the increase of open circuit voltage, and thus reduce the solar cell efficiency. Here, we introduce quercetin, a phenolic derivative with antioxidation properties extracted from plants, as the additive to reduce the existence of Sn4+ and prevent the FASnI3 film from degradation. We use grazing-incidence wide-angle X-ray scattering (GIWAXS) to gain insights into the detailed steps of growth and degradation progress of the active layer. Thereby, GIWAXS offers a way to gain information about the time evolution during the crucial steps of interface formation.

CPP 28.36 Wed 11:30 Poster C

Tuning band gap of double perovskite by anion exchange — •Zhaonan Jin[1] and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]TUM, MLZ, 85748 Garching, Germany

Double perovskite is a relatively new kind of lead-free perovskite that possesses low toxicity, long charge carrier lifetime and small effective charge carrier mass. It is considered as a promising photovoltaic material. Bismuth-based double perovskites have received considerable attention in recent years, and among them, Cs2AgBiX6 (X =Cl, Br, I) has displayed the most promising potential for photovoltaic applications due to the suitable band gap. Some researchers studied thermoelectric properties of double halide perovskite Cs2AgBiI6 and proved that it is an excellent candidate for thermoelectric applications. Increasing the content of iodide ions in Cs2AgBiX6 can effectively narrow the band gap. In this work, the iodide ions will be introduced to Cs2AgBiBr6 by adding TMSI when spin-coating. It is reported that no more anion exchange happened with more TMSI. Therefore, Cs2AgBi(BrxI1-x)6 perovskite solar cells will be fabricated by solution method. The anion exchange process is studied in this work. Morphology, device characterizations techniques like XRD, SEM, J-V curves, EQE spectra etc. are taken to help optimize the morphology of thin films and PCE of solar cells. In-operando studies are taken to identify morphology changes during device operation.

CPP 28.37 Wed 11:30 Poster C

Effect of Additives on Dion-Jacobson Two-Dimensional Perovskite Solar Cells — •Kin Long Fong[1], Kun Sun[1], and Peter Müller-Buschbaum[1,2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]TUM, MLZ, 85748 Garching, Germany

Solar cells based on two-dimensional (2D) perovskite materials have received more attention in recent years due to their stability compared to their three-dimensional counterparts. However, their power conversion efficiencies (PCEs) are still lagging behind, posing a major challenge before their commercialization. In this work, we study the effects of additives, namely MACl, PbCl2, and a mixture of MACl and PbCl2, on the structures of Dion-Jacobson (DJ) 2D perovskite films fabricated with 1,4-phenylenedimethanammonium (PDMA) spacer molecules. Solar cells made with these films are also investigated, and their efficiencies are presented. This research aims to enhance our understanding of the impact of different additives on the PCEs of solar cells based on PDMA spacers.

CPP 28.38 Wed 11:30 Poster C

Exploring the potential of lead halide perovskite as materials with high stokes shift for photovoltaic applications — •Elshaimaa Darwish, Jack Elia, Andres Osvet, Miroslaw Batenbatentschuk, and Christoph Brabec — i-MEET Institute Materials for Electronics and Energy Technology, Erlangen

Lead halide perovskites has been attracting a lot of research interest over the past years. Due to the unique properties of lead halide perovskites such as high defect tolerance, high absorption coefficient and tunable band gab, they are considered a highly promising class of materials for optoelectronic devices and photovoltaics. One of the issues that is hindering the perovskites application is possessing small stokes shifts or self-absorption. Therefore, developing lead halide perovskites with large stokes shifts is a significant venture.

There are a number of approaches used to control the stoke shifts in semiconductors including chemical composition, size, temperature, and other reaction conditions. In this work, structural modifications were introduced into inorganic lead halide perovskite as a way of obtaining high stoke shift, we characterize the obtained particles optically, and structurally. Moreover, scanning electron microscope (SEM) was used to measure the change in particle size as a result of introducing modifications.

The successful incorporation of the synthesized particles into transparent or semitransparent films could be used to enhance the performance of the currently available solar cells in the market.

CPP 28.39 Wed 11:30 Poster C

Charge transfer and recombination in hole transport/perovskite bilayers probed by photoluminescence — •Lukas Schäfer, Patrick Dörflinger, Olga Trukhina, and Vladimir Dyakonov — Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

Hole transport materials (HTMs) play a crucial role in enhancing the performance of perovskite solar cells by selectively extracting holes from the active layer. While their charge extraction capabilities positively impact solar cell efficiency, surface recombination at the perovskite interface can hinder overall performance. In this study, we employ steady-state PL (SSPL) as well as time-resolved PL (TRPL) experiments on HTM/perovskite bilayers to assess the charge extraction capability and the surface recombination. We demonstrate the quenching of the photoluminescence quantum yield of these bilayers which is characteristic for the extraction of charges and their non-radiative recombination at the HTM/perovskite interface. Furthermore, the bilayers exhibit a faster decay in TRPL transients compared to pristine perovskite. This can be indicative for charge extraction and surface recombination. SSPL and TRPL have proven to be useful tools to characterize novel HTMs for perovskite solar cell applications and to gain insights into the processes at the interface between the perovskite and the HTMs.

CPP 28.40 Wed 11:30 Poster C

Influence of additives on the recombination dynamics in lead-halide perovskite absorbers probed by TRMC and SSMC — •Mechthild Seidl[1], Patrick Dörflinger[1], Mohammad Khaja Nazeeruddin[2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany — [2]Group of Molecular Engineering of Functional Materials, Institute of Chemical Sciences and Engineering, EPFL Valais, Sion 1950, Switzerland

Perovskites have attracted attention due to the possibility of using them as a top cell with a wide bandgap in tandem solar cells. However, a significant challenge associated with perovskites is their instability. One promising approach to enhance their performance and stability involves the incorporation of additives. Two contactless measurement techniques, time-resolved microwave conductivity (TRMC) and steady-state microwave conductivity (SSMC) are used to characterize and understand the influence of the additives. Both techniques uses the interaction of light-induced charge carriers with an electromagnetic field inside a cavity to measure a change in conductance. SSMC provides insight into the dominant charge carrier recombination pathway, while TRMC is employed to determine the mobility and lifetime of generated charge carriers in the perovskite. An understanding of the influence of the additives on these optical properties is essential to improve the solar cell's performance further.

CPP 28.41 Wed 11:30 Poster C

Monolithic series interconnection of perovskite CIGSe tandem modules by laser patterning: Process development and material characterization — •Nicolas Otto[1], Christof Schultz[1], Guillermo Farias-Basulto[2], Oliver Fischer[3], Rutger Schlatmann[1,2], Eva Unger[4], and Bert Stegemann[1] — [1]HTW Berlin - University of Applied Sciences, Wilhelminenhofstr. 75a, D-12459 Berlin, Germany — [2]PVcomB / Helmholtz-Zentrum Berlin für Materialien und Energie, Schwarzschildstr.3, D-12489 Berlin, Germany — [3]Fraunhofer Institute for Solar Energy Systems ISE, Heidenhofstr. 2, 79110 Freiburg, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, Young Investigator Group Hybrid Materials Formation and Scaling, Kekuléstraße 5, D-12489 Berlin, Germany

Perovskite and chalcopyrite based solar cells for 2-T tandem devices enables efficiencies beyond the SQ limit for single junction cells. Both materials can be electrically interconnected by monolithic series interconnection, which comprises alternating layer deposition and layer patterning steps (P1, Isocut, P2, and P3). The goal is to develop suitable patterning parameters for each of the four scribe lines by systematic variation of the laser fluence. Suitable process windows were determined by analyzing the electrical functionality of the scribe lines, their geometry (using laser-scanning microscopy), and photo-activity (using intensity dependent photoluminescence imaging of the individual subcells) as well as alterations in the material composition in the scribe line vicinities (using energy-dispersive x-ray spectroscopy, EDX).

CPP 28.42 Wed 11:30 Poster C

Temperature Dependent Photoluminescence Studies of Metal-Free Phthalocyanine Single Crystals — •Luise Pätzold[1], Lisa Schraut-May[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]CAE Bayern, 97074 Würzburg

The opto-electronic properties of organic materials depend not only on the individual molecules, but also on their interaction in the crystalline lattice [1]. As a representative, the material class of phthalocyanines (Pc) is studied in various research fields because of the possibility to steer its opto-electronic and structural properties by choice of the central metal atom, chemical substitution of its periphery and, thus, aggregate packing [2]. This distinguishes Pc compounds to investigate the excitonic coupling between neighboring molecules under various conditions. We have grown β-phase single crystals of metal-free H_2-phthalocyanine (H_2-Pc) by horizontal vapor phase deposition. Polarization dependent photoluminescence (PL) measurements provide insights into the anisotropic coupling of the photoexcited molecules within the crystallographic ($\bar{1}01$) plane. Furthermore, changes in the excitonic coupling are investigated as function of temperature down to 5 K. The results will be discussed in comparison to metal-centered zinc-phthalocyanine (Zn-Pc), where a super-radiant PL enhancement is observed below 80 K which is related to a discontinuous change in inter-molecular coupling at cryogenic temperatures.

[1] Hestand et al., Chem. Rev. (2018)

[2] Rödel et al., J. Phys. Chem. C (2022)

CPP 28.43 Wed 11:30 Poster C

Influence of the Atmosphere on the Phosphorescence of a Brominated Diphenylphosphine Oxide–Ethyl Naphthaleneimide Dyad — Marvin Malchau[1], Paul M. Reichstein[2], Werner Reichstein[3], and •Lothar Kador[1] — [1]University of Bayreuth, Institute of Physics and BIMF, 95440 Bayreuth, Germany — [2]University of Bayreuth, Macromolecular Chemistry I and BIMF, 95440 Bayreuth, Germany — [3]University of Bayreuth, Bayreuth Materials Center (BAYMAT), 95440 Bayreuth, Germany

The non-brominated diphenylphosphine-ethyl naphthaleneimide dyad (DPPENI) acts as a sensitive sensor for cumulative exposure to oxygen, since, under simultaneous irradiation of UV or blue light, the diphenylphosphine unit is oxidized to diphenylphosphine oxide; as a consequence, blue fluorescence emission is turned on in the originally non-fluorescing compound. [1] Upon bromination of the naphthaleneimide unit, strong phosphorescence is emitted in addition to the fluorescence. We studied the intensity and lifetime of the phosphorescence of the fully oxidized Br-DPPENI dyad in atmospheres of air, argon, helium, nitrogen, and oxygen as a function of pressure between vacuum and 1 bar. The experiment was performed in the frequency domain with a two-channel lock-in amplifier and the data were analyzed with the polar-plot or phasor technique. Reversible phosphorescence quenching due to triplet-triplet annihilation was found in the presence of atmospheric or pure oxygen, whereas the other gases had no effect.

[1] R. Shritz et al., Chem. Eur. J. **21**, 11531 (2015).

CPP 28.44 Wed 11:30 Poster C

Intramolecular Barrier for Stilbene Photoisomerization from Temperature- and Viscosity-Dependent Transient Absorption — •Daria Schriever[1], Alexander L. Dobryakov[2], J. Luis Perez Lustres[1], Martin Quick[3], Ilya N. Ioffe[4], and Sergey A. Kovalenko[3] — [1]Fachbereich Physik, Freie Universität Berlin — [2]Moscow — [3]Institut für Chemie, Humboldt Universität zu Berlin — [4]Moscow

The photoisomerization of stilbene is investigated by means of fs broadband transient absorption in solution and compared to the RRKM and Kramers reaction rate theories [1]. To this end, it is necessary to extract the intramolecular barrier from the experimental one, which contains the viscosity contribution. Reaction dynamics is measured in a range of temperatures and non-polar solvents of various viscosities. In this way, the barrier height remains virtually unaffected by polar interactions between the surrounding solvent and the polar transition state of the isomerization reaction. In parallel, viscosity activation energies are obtained from the rotational diffusion times of the stilbene molecule. It is found that the isomerization time constant is proportional to η^{α}, with $\alpha = 0.3$. An average barrier of 1236 cm^{-1} is obtained, in good agreement with the gas phase results: 1398 cm^{-1} [2].

[1] S. A. Kovalenko, A. L. Dobryakov, *Chem. Phys. Lett.* **2013**, *570*, 56-60. [2] J. S. Baskin *et al*, *J. Phys. Chem.* **1996**, *100*, 11920-11933.

CPP 28.45 Wed 11:30 Poster C

Extension of parametrization for long-range corrected DFTB and its application on organic photovoltaics — •Wenbo Sun[1], Tammo van der Heide[1], Carlos R. Lien-Medrano[1], Thomas Frauenheim[2], and Bálint Aradi[1] — [1]University of Bremen, Bremen 28359, Germany — [2]Constructor University, Bremen 28759, Germany

In recent years, the field of organic photovoltaics (OPV) has witnessed significant progress, marked by the synthesis of novel donor and acceptor molecules. To gain deeper insights into the mechanisms of OPV and predict the electronic properties of molecules, theoretical computational methods are frequently employed. However, the application of Density Functional Theory (DFT) calculations faces limitations when dealing with large systems, such as dimers of donor-acceptor molecules or aggregates, due to their computational requirements. As an alternative, the Density Functional Tight Binding (DFTB) method is an approximation to Kohn-Sham DFT, usually being orders of magnitudes faster. For the description of charge transfer excited states by DFTB, the incorporation of long-range corrected hybrid functionals into DFTB (LC-DFTB) becomes essential.

Based on the existing ob2-1-1 parameter set [1] containing the chemical elements C, H, N, and O, the present work extends these parameters to include S, F, and Cl. The extension of parametrization broadens the scope for investigating novel OPV molecules via LC-DFTB, such as non-fullerene acceptor Y6, as well as small-molecule donors BTR and BTR-Cl, along with their respective dimers and aggregates.

[1] J. Chem. Theory Comput., 2018, 14, 115-145.

CPP 28.46 Wed 11:30 Poster C

Behaviour of metal-containing films of chitosan-based films in aqueous solutions — •Snegireva Anastasia — Moscow, Russia

The behaviour of biologically active coating materials in aqueous solutions is an important feature for determining the area of application and the possibility of use as a drug. The dynamics of the change in these parameters over time under standard conditions for storing the materials determines one of the parameters for the shelf life of the foils obtained. Films containing iridium and rhodium were produced by the solution casting method. There are three types of films: chitosan-based, chitosan-gelatin-based and chitosan-agar-based. The degree and the swelling constant were determined both in aqueous solution and in salt buffer solution with a pH value of 7.2, which corresponds to the ion set and the acidity of the organism's biological media. The addition of metal cations to the films changes the character of the solution. Matrices that do not contain salt swell without restriction in both aqueous and buffer solutions. As the metal concentration in the foils increases, the degree of swelling decreases. The swelling rate constant increases. The ability to absorb moisture during storage under standard conditions decreases over a period of two months, which indicates an increase in the strength of the materials.

CPP 28.47 Wed 11:30 Poster C

Light-Driven Charge Regulation at Oil/Water Interfaces in Nanoemulsions

— •Dana Glikman and Björn Braunschweig — Institute of Physical Chemistry and Center for Soft Nanoscience, University of Münster, Busso-Peus-Str. 10, 48149 Münster

Understanding oil/water (o/w) interfaces in nanoemulsions and on a molecular level is of great interest, but often impaired by experimental limitations to probe the internal interfaces in situ. In order to study and to tune nanoemulsions we make use of photoswitchable surfactants. For that we apply arylazopyrazole sulfonate (butyl-AAP) surfactants which can be photoisomerized between E and Z isomers by visible and UV light. This causes massive changes in the interface tension at the extended o/w interface and a drastic shift in the surfactants' CMC, which we apply to control the stability of the macroemulsions through UV irradiation. Nanoemulsions with a droplet radius of 90 nm were, however, not susceptible to E/Z photoisomerization in terms of changes in particle size or in the ζ-potential. However, second-harmonic generation in the scattering mode (SHS) shows that the surfactants' surface excess at the nanoscopic o/w interface is changed drastically and reversibly by E/Z photoisomerization. The apparent differences in the ζ-potential and the changes in surface excess provide evidence for a fixed charge to particle size ratio and the need for counter ion condensation in order to renormalize the particle charge to a critical charge per particle, which is largely different to extended interfaces.

CPP 28.48 Wed 11:30 Poster C

Time-dependent morphology evolution of templated mesoporous titanium films

— •Guangjiu Pan[1], Tianle Zheng[1], Suzhe Liang[1], Altantulga Buyan-Arivjikh[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

Mesoporous transition metal oxides have attracted significant interest due to their excellent properties. The soft templating approach with the sol-gel method is one of the most common approaches for designing mesoporous transition metal oxides. However, the influence of hydrolysis and condensation of precursors on the morphology is still unclear. Commercial metal alkoxide precursors were chosen in this work to demonstrate the influence of the reaction time. A similar morphology transition, from worm-shaped mesopores to ordered spherical mesopores, was observed with increasing sol-gel reaction time for different precursors. The surface morphologies of spin-coated films are probed via scanning electron microscopy and grazing-incidence small-angle X-ray scattering (GISAXS).

CPP 28.49 Wed 11:30 Poster C

Photo-thermal Expansion of Nanostructured Surfaces in Photoinduced Force Microscopy (PiFM)

— •Shohely Anindo[1,2], Jesvin Joseph[2,3], Rainer Heintzmann[2,3,4], Daniela Täuber[3,4], and Christin David[1,2] — [1]IFTO, Friedrich Schiller University Jena — [2]Abbe Center of Photonics, Jena — [3]Leibniz Institute of Photonic Technology, Jena — [4]Institute of Chemical Physics, Friedrich Schiller University Jena, Germany

The recently developed Photo-induced Force Microscopy (PiFM) offers high spatial resolution in chemical imaging of polymer films and biomaterials, when combined with mid-infrared illumination. Upon absorption, photo-thermal expansion of the material causes a modulation of the Van der Waals (vdW) force acting between the tip and the sample. This work theoretically investigates the non-linear impact of material properties and surface shape on the tip-sample interaction, heat generation from the presence of a photo-induced electric field, the resulting thermal expansion under different illumination conditions and the change in cantilever oscillation at different detection modes. We compare our results to mid-infrared PiFM images obtained from a poly(methyl methacrylate) (PMMA) nanosphere with a diameter of 100 nm.

CPP 28.50 Wed 11:30 Poster C

Influence of Polymers on Ice-Polymer Premelting Dynamics

— •Takumi Sato[1], Ikki Yasuda[1], Yusei Kobayashi[2], Noriyoshi Arai[1], and Kenji Yasuoka[1] — [1]Keio University, Kanagawa-ken, Japan — [2]Kyoto Institute of Technology, Kyoto, Japan

As exemplified by ice rinks, even at temperatures below the freezing point, the ice surface undergoes melting, forming a pseudo-liquid layer known as the premelting layer. Such a premelting layer is generated not only at the ice-vapor interface but also at the ice-polymer (rubber) interface, significantly influencing the properties of the ice surface. Extensive research has been conducted on the premelting layer, which has been observed at the ice-vapor interfaces. However, the behavior of the premelting layer at the ice-polymer interface has not been clarified.

Understanding the behavior of the premelting layer at the ice-polymer interface, is considered to make a substantial contribution to the development of applications such as winter tires for automobiles. However, clarifying the behavior of the premelting layer at the ice-polymer interface due to friction is challenging, given the variability under numerous conditions such as temperature, pressure, velocity, and the surface roughness of the rubber.

In this study, we initiate all-atom molecular simulations at the ice-polymer interface using polymers such as polyethene. This allows us to analyze the molecular dynamics of the premelting layer, revealing the influence of polymers on the premelting layer and elucidating the physical properties of the premelting layer.

CPP 28.51 Wed 11:30 Poster C

Advancing Microscopy Techniques for Plastic Analysis in Transmission Electron Microscope and Focused Ion Beam

— •Judith Bünte, Inga Ennen, Laila Bondzio, and Andreas Hütten — Universität Bielefeld, Dünne Schichten und Physik der Nanostrukturen, Universitätsstr. 25, 33615 Bielefeld, Germany

Plastics play an essential role in various industries. Wanting to reduce plastic waste their analysis is necessary for advancing high-quality recyclate usage. While it is easy to downcycle pre-used plastics, we do not want to lose product quality in the recycling process. Here, we present our workflows for plastic analysis using Transmission Electron Microscope (TEM) and Focused Ion Beam (FIB) techniques. The goal is to explore diverse contrast enhancement techniques to unravel complex details of plastic structures. Understanding these structures is important for optimizing recyclate usage.

Our toolbox of experimental setups employs state-of-the-art TEM and FIB technologies, providing high-resolution insights into the morphology and composition of plastics. By investigating and comparing contrast enhancement methods, we aim to refine the imaging process and contribute to a more comprehensive understanding of plastic materials.

CPP 28.52 Wed 11:30 Poster C

Investigation of the impact of dissolved H2 on the surface properties of ionic liquids

— •Arsha Cherian[1], György Hantal[1], Christian Wick[1], and Ana-Sunčana Smith[1,2] — [1]PULS Group, Institute for Theoretical Physics, IZNF, FAU Erlangen- Nrnberg, 91058 Erlangen, Germany — [2]Group for Computational Life Sciences, Ruder Bošković Institute, Bijenička 54, HR-10000 Zagreb

SILP (Supported Ionic Liquid Phase) catalysis technology focuses on obtaining a heterogenised type of homogeneous catalytic systems where a thin film of ionic liquid (IL) containing a homogeneous catalyst is immobilised on the surface of a porous support material, which is commonly employed in hydrogen-involved catalysis systems. The dissolution of small, non-polar molecules of hydrogen in the ionic liquid film resulting in highly asymmetrical system in terms of molecular structures, is expected to have an influence in the thermophysical properties of IL which can subsequently affect the reaction kinetics and ultimately impact the overall reaction rate. In order to understand this influence of dissolved hydrogen on the surface properties of ILs, molecular dynamics (MD) simulations were conducted using GROMACS software in binary mixtures consisting of an ionic liquid (IL) with pressurized molecular hydrogen, between 298 and 393K over a broad pressure ranging from 1 to 30 MPa. We find that the addition of H2 results in a decrease in the surface tension of both binary mixtures up to about 6 percent at higher pressures, which is more pronounced at lower temperatures. Furthermore, an enrichment of hydrogen is observed at the liquid-gas interface of these binary mixtures.

CPP 28.53 Wed 11:30 Poster C

Charge characterization of latex colloids under thoroughly deionized and decarbonized as well as under ambient CO_2 conditions

— •Peter Vogel and Thomas Palberg — Johannes Gutenberg Universität, Mainz, Germany

We report on the charging behavior of dielectric colloidal particles bearing dissociable surface groups in salt-free aqueous environments in absence and presence of ambient CO_2. We performed systematic measurements of the low-frequency bulk conductivity in dependence on the particle number density and upon adding neutral electrolytes to determine both the effective and bare particle charges based on our conductivity model assuming independent migration of all ionic species present in solution. We find that upon equilibration with ambient CO_2 the effective number of freely mobile counterions decreases by about 50 %. As function of the electrolyte concentration, the measured conductivity reveals a pronounced difference in the curve shape depending on the presence of CO_2. Caused by the surface adsorption of molecular CO_2, we demonstrate the absence of micro-ionic exchange processes in-between the proposed inner and outer part of the electrical double layer as deviated from the strict linear increase in conductivity. Conversely, starting from the deionized and decarbonized state, we observe a pronounced non-linear behavior fully accounted for by our model assumptions.

CPP 28.54 Wed 11:30 Poster C

Fast on-chip AC Seebeck measurement — •Andreas Waxweiler, Ejona Syla, Clara Wiesner, Morteza Shokrani, and Martijn Kemerink — Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University, 69120 Heidelberg, Germany

Organic thermoelectric generators (OTEGs) show promise as a renewable energy source for small-scale devices. Despite the growing emphasis on improving the Seebeck coefficient (S) of organic materials, a precise and fast measurement of S of organic thin films appears to be lacking: the common DC method for measuring S involves substantial waiting times and must be repeated for multiple temperature gradients, which makes the measurement slow and prone to errors. To overcome this, we propose a fast, robust and easy-to-calibrate Seebeck coefficient measurement utilizing an alternate current (AC) technique. In this method, an oscillating current (frequency ω) is applied to an on-chip thin film heater. The resulting thermal wave (frequency 2ω) leads to an AC thermovoltage at the same frequency that is measured by lateral electrodes across the chip. The solution of the 1-dimensional heat equation aligns well with the experimentally measured temperatures at the electrodes, allowing us to be independent of temperature measurements by calibrating the system with the heat equation. As a result, our system requires neither an external heater or cooler, nor a temperature sensor. The measurement times can be drastically decreased to less than a minute, using a chip design that can be fabricated by simple thermal evaporation through a shadow mask.

CPP 28.55 Wed 11:30 Poster C

The Mueller Matrix for Scattering by Polydisperse Non-Chiral Samples — •Reinhard Sigel — 88677 Markdorf, Germany

Light scattering measurements at a thin film or by an ensemble of particles in a dispersion are versatile tools for sample characterization. To fully exploit the technique for maximum information, the control of polarization of the incident and the detected light is required. Often samples are not ideal but include distributions of the orientation of anisotropic scattering centers and their sizes. Thus, a theoretical description ends up in the Stokes-Mueller formalism [1]. All 16 elements of the Mueller matrix can be measured [2]. It remains a task, however, to make use of such a set of partially interdependent data for a characterization of the sample which produces such scattering. The simplest case are samples without depolarization, where there is no intermixing between two orthogonal linear polarization directions. A size distribution of isotropic scattering centers is sufficient to fit an experimental Mueller Matrix for such a case [3]. To extend the model to depolarization in the simplest case, we assume equal scattering behavior for left and right circularly polarized light. Such equality is to be found for non-chiral samples. It reduces the number of independent parameters, and it is sufficient to consider a common polydispersity distribution of two real parameters for the resulting Mueller matrix.
[1] C.F.Bohren, D.R. Huffman, *Absorption and Scattering of Light by Small Particles* (Wiley, Weinheim 1983).
[2] R.M.A. Azzam, Opt. Lett. 2, 148-150 (1978).
[3] R. Sigel, A. Erbe, Appl. Opt. 47, 2161-2170 (2008).

CPP 28.56 Wed 11:30 Poster C

Significant reduction in electrical conductivity of PEDOT:PSS with new Schiff base salts additives — •Ameneh Mikaeeli[1,2], Nathan Jukam[2], Anna Kmieciak[3], Robert Szczesny[3], Arne Ludwig[2], Bayram Gunduz[4], Andreas D. Wieck[2], and Michal Pawlak[1] — [1]Faculty of Physics, Astronomy, and Informatics, Nicolaus Copernicus University in Torun, Grudziadzka 5, 87-100 Torun, Poland — [2]Chair of Applied Solid-State Physics, Faculty of Astronomy and Physics, Ruhr-University Bochum, D-44780, Bochum, Germany — [3]Faculty of Chemistry, Nicolaus Copernicus University in Torun, Gagarina 7, 87-100 Torun, Poland — [4]Malatya Turgut Ozal University, Faculty of Engineering and Natural Sciences, Department of Engineering Basic Sciences, 44210 Malatya, Turkey

PEDOT:PSS layers were prepared with three different additives. In particular, the conductivity effects of additives on PEDOT:PSS layers were examined depending on temperature. The conductivity values of PEDOT:PSS layers increase significantly with increasing temperature. These results confirm that PEDOT:PSS exhibits semiconductor properties. Additionally, there appears to be a significant difference, although not a vast difference between the conductivities of PEDOT:PSS for the three different additives. All these results show that both additives and especially temperature change the conductivities of PEDOT:PSS.

CPP 29: Gels, Polymer Networks and Elastomers II

Time: Wednesday 15:00–16:15 Location: H 0106

CPP 29.1 Wed 15:00 H 0106

Structural characterization of model gels at preparation conditions and at swelling equilibrium — •Michael Lang and Reinhard Scholz — Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany

We use large scale computer simulations of star polymer model gels to separate the static and the dynamic contributions of the scattering intensity $I(q)$, allowing to determine the correlation length ξ of the corresponding polymer solution and the static correlation length Ξ combining several properties of the denser cross-link blobs. The correlation length ξ can incorporate parts of the form factor of the stars for polymer volume fractions around the overlap condition of the stars, affecting a determination of ξ from the scattering data. At swelling equilibrium, the cross-link motion is confined within a volume comparable to the size of the somewhat denser cross-link blob. Since the cross-link blob size scales $\propto \xi$, we measure $\Xi \propto \xi$ for our near ideal model networks. The confined motion of the cross-links implies a Gaussian shape for the static contribution. At swelling equilibrium, the dynamic part of the scattering intensity $I_{\rm dyn}(0)$ related to the solution-like correlation lengths is almost identical to the scattering intensity $I_{\rm stat}(0)$ of the static part. At preparation conditions, $I_{\rm stat}(0)/I_{\rm dyn}(0)$ decays with a power law following the polymer fraction of the cross-link blobs. Here, the larger volume available volume for cross-link motion stands out for increasing polymer volume fraction, reducing the concentration dependence of Ξ.

CPP 29.2 Wed 15:15 H 0106

Nonlocal elasticity explains equilibrium patterns in gels induced by phase separation — •Yicheng Qiang, Chengjie Luo, and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

Recent experiments found regular patterns in elastic gels, which emerged during cooling-induced phase separation. The patterns form without hysteresis, suggesting a continuous phase transition. To understand these observations, we propose an equilibrium field-based model based on phase separation between an elastic component and the solvent, augmented by nonlocal elasticity, which captures the microstructure of the gel. The model reveals a continuous phase transition from a homogenous state to patterns in stiff gels. Analytical approximations demonstrate that the pattern period is proportional to the geometric mean between the elasto-capillary length and a microscopic length scale of the gel, in good agreement with experimental observations. Our theory highlights the importance of nonlocal elasticity in soft matter systems, reveals the mechanism of equilibrium mesoscopic patterns due to elasticity, and will improve the engineering of such materials with controlled mesoscopic structure.

CPP 29.3 Wed 15:30 H 0106

Probing the microstructure properties of soft magnetic polymer hybrid materials using simulations — •Chinmay Pabshettiwar, Patrick Kreissl, Christian Holm, and Rudolf Weeber — Institute for Computational Physics, University of Stuttgart(US)

Embedding magnetic nanoparticles within a polymer hydrogel results in materials combining magnetic and viscoelastic properties, making them promising candidates for engineering and biomedical applications[1, 2]. Due to wide range of applications, it is essential to understand the coupling between magnetic nanoparticles and polymers and its effect on mechano-elastic properties. Experimentally, this is studied by analyzing the frequency-dependent magnetic susceptibility. In our study, we model this approach using computer simulations combining coarse-grained molecular dynamics and Lattice-Boltzmann hydrodynamics. Using such simulations, it is possible to switch on specific interactions, such as magnetic, steric, van der Waals, or hydrodynamic, individually. Hence, their influence on nanoparticle-polymer coupling can be studied. Using this technique, in our contribution, we study the effect of the hydrogel's mesh size on the magnetic relaxation behaviour of the nanoparticles. We compare different interaction potentials between the nanoparticle and the polymer chains. Furthermore, we obtain the AC susceptibility spectrum from the Green-Kubo approach[3] by analyzing the thermal fluctuation spectrum of magnetization in the absence of an external field.

References : [1] Filipcsei et al., 2010 [2] Weeber et al., 2018 [3] Kreissl et al., 2021

CPP 29.4 Wed 15:45 H 0106

Structure-Property Relationships of Biobased High-Performance Vitrimers — •Paulina Szymoniak[1], De-Yi Wang[2], and Andreas Schönhals[1] — [1]Federal Institute for Materials Research and Testing (BAM) Unter den Eichen 87, 12205 Berlin, Germany — [2]IMDEA Materials Institute, Eric Kandel 2, 28906 Getafe, Madrid, Spain

Epoxy vitrimers are a novel class of materials, showing great potential as sustainable replacement to classical epoxy thermosets within the frames of circular economy. Vitrimers are based on covalent adaptive networks (CANs), where dynamic bonds can break/reform and reshuffle upon a suitable stimulus, endowing polymers with unprecedented properties, such as shape-memory, self-healing, and recyclability. Here, the relationships between the microscopic structure and molecular mobility with thermomechanical performance of a novel vitrimer are studied. The material is based on glycerol triglycidyl ether (GTE) and vanillin-derivative hardener (VA), which represents an ideal biobased substitute for fossil-derived epoxy resins. The applied methodology comprises X-ray scattering, dielectric and mechanical spectroscopy, as well as calorimetry. Dielectric investigations of the materials revealed two dielectrically active processes, i.e., one related to segmental mobility, and a second broad process related to topology reshuffle. Further, GTE-VA is considered in the 'as-prepared' and 'healed' state, where the thermomechanical properties are studied as a function of recycling cycles, showing weak dependency on the healing procedure.

CPP 29.5 Wed 16:00 H 0106

Structural characterization of amphiphilic star polymer conetworks — •Reinhard Scholz[1], Michael Lang[1], Lucas Löser[2], and Kay Saalwächter[2] — [1]Leibniz Institut für Polymerforschung, Hohe Str. 6, 01069 Dresden, Germany — [2]Institut für Physik - NMR, Betty-Heimann-Str. 7, Martin-Luther Univeristät Halle-Wittenberg, 06120 Halle, Germany

We analyze the structure of amphiphilic polymer co-networks consisting of hetero-complementary bound four functional star polymers A_4 and B_4 by computer simulations and by SAXS measurements. The computer-generated networks were characterized in an a-thermal cosolvent and in an increasingly poor solvent for the B component. In the poor solvent regime, the calculated pair distribution reveals a long-range radial oscillation, corresponding to the formation of dense B clusters and a pronounced peak in the scattering intensity. All simulated scattering data are decomposed into scattering from the time average density and from thermal fluctuations around this background, revealing an increased correlation length around the phase transition. Polymer networks consisting of complementary four functional stars of poly ethylene glycol (PEG) and poly caprolactone (PCL) were synthesized via covalent coupling of complementary end groups. Their SAXS data in different solvents were analyzed with a combination of model functions deduced from the computer simulations, revealing excellent agreement between observed and simulated length scales of the nanophase separation.

CPP 30: Charged Soft Matter, Polyelectrolytes and Ionic Liquids II

Time: Wednesday 15:00–18:00 Location: H 0107

CPP 30.1 Wed 15:00 H 0107

Dimensionality Effects in the Tuning of Thermoelectric Transport Properties of Polymer Electrolytes by Carbon-based Additives — •Julian-Steven Schilling, Maximilian Frank, Theresa Zorn, Philipp Kessler, Ivonne Vollert, Tobias Hertel, Ann-Christin Pöppler, and Jens Pflaum — University of Würzburg, 97074 Würzburg

The abundance of their chemical constituents, their solution-based processing in combination with the inherently low thermal conductivity have propelled polymers to the forefront of organic thermoelectrics. Since ionic systems exhibit significantly higher thermal voltages than electronic materials, a combinations of material classes seems to be very promising. This study extends our previous findings [1] on the thermoelectric transport properties of a methacrylate-based solid polymer electrolyte prepared by solution processing by new data obtained by changing the conducting salt from LiTFSI to NaTFSI. Employing impedance spectroscopy across a wide frequency range (100 mHz to 510 kHz) together with thermoelectric voltage measurements at technologically relevant temperatures from 263 K to 353 K, we highlight the main concentration-dependent differences resulting from utilization of NaTFSI instead of LiTFSI as conducting salt. Additionally, we demonstrate the potential of tailoring the transport properties of these solid state polymer electrolytes by incorporating carbon-based additives of different dimensionality (1D or 2D) and conductivity characteristics (semiconducting or metallic). [1]M. Frank, et al., Adv. Funct. Mater. 32 (2022) 2203227

CPP 30.2 Wed 15:15 H 0107

Ion dynamics and resonance in an electrical double layer undergoing periodic excitation by a surface acoustic wave — Sudeepthi Aremanda, Oles Dubrovsky, and •Ofer Manor — Technion - Israel Institute of Technology, Haifa, Israel

Electrical double layers (EDLs) appear at the interface between charged surfaces and electrolyte solutions and are one of the most fundamental and abundant mechanisms in nature. Steady and quasi-steady measurements of EDL properties are commonplace. However, the EDL Debye length, measured in nanometers, and the ion relaxation time through the Debye length, measured in nanoseconds, have made measurements of ion dynamics inside EDLs elusive.

We capture EDL dynamics by imposing a field effect, an evanescent mechanical wave generated in an electrolyte solution by a MHz-frequency surface acoustic wave (SAW) traveling in a neighboring substrate. Ions in the EDL undergo mechanical vibrations at the SAW frequency and support a same frequency leakage of alternating electrical field off the EDL that we measure. Moreover, a SAW excitation frequency comparable to the inverse of an ion relaxation time supports electro-mechanical ion resonance. The latter maximizes the ion mechanical vibration and the magnitude of the electrical field leakage, rendering ion-specific relaxation times measurable and giving the intrinsic rate of EDL charge and discharge by specific ions. [1]

[1] S. Aremanda and O. Manor, J. Phys. Chem. C, 2023, 127, 20911-20918

CPP 30.3 Wed 15:30 H 0107

Attractive Interactions of Eco-corona Covered Microplastic Particles in Aqueous Environment — •Thomas Witzmann[1], Günter Auernhammer[1], Andreas Fery[1,2], Simon Wieland[3], and Holger Kress[3] — [1]Leibniz Institute of Polymer Research Dresden — [2]Physical Chemistry of Polymeric Materials, Technische Universität Dresden — [3]Biological Physics, University of Bayreuth

Microplastic particles in the environment are covered by a so-called eco-corona. The eco-corona is made up of natural organic matter (NOM) like biomolecules, humic substances and other natural molecules. NOM changes the surface properties of microplastic particles and therefore the interaction with other surfaces in the aqueous environment influencing their aggregation behaviour. Using Colloidal Probe-AFM we studied the interactions of eco-corona covered microplastic particles. Measurements were performed in different ionic concentrations to mimic changing environmental conditions and to step-wise reduce electrostatic contributions. We found that the eco-corona is able to "pull" at the colloidal probe by polymer bridging. This bridging energy decreases with increasing eco-corona coverage of the probe surface. Bridging was present at 1, 10 and 150 mM KCl. No bridging occurred at 0.1 mM KCl. In conclusion, we show that the eco-corona is able to form polymer bridges and "pull" surfaces towards itself. This mechanism may contribute substantially to microplastic aggregation in the aqueous environment.

CPP 30.4 Wed 15:45 H 0107

Exploring ATP-Zn^{2+} complexes in water with IR spectroscopy: experiments and ab initio simulations — •emma rossi[1,3], achintya kundu[2], thomas elsaesser[2], marialore sulpizi[3], and alberta ferrarini[1] — [1]Università degli Studi di Padova, Padova, Italy — [2]Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Berlin, Germany — [3]Ruhr Universität Bochum, Bochum, Germany

ATP-Zn^{2+} complexes are of significant interest for several applications, including the design of self-assembling systems and catalysis. Understanding the mechanisms behind these applications requires a clear structural characterization of ATP-Zn^{2+}. This problem is far from trivial since the presence of charges, highly polarizable species, water and the conformations of the triphosphate chain lead to a wide variety of possible geometries. To elucidate the structure of ATP-Zn^{2+} complexes, we experimentally measured the IR absorption spectra of ATP in water both in the absence and presence of Zn^{2+}. Accurate band assignments were performed by comparing the experimental spectra with simulated IR spectra of methyl triphosphate (MTP), a simplified model for ATP, and MTP-Zn^{2+} complexes in a few selected coordination modes. The spectra were obtained through ab initio molecular dynamics trajectories and the time-correlation function method. Using this approach we identified the coordination modes of the ATP-Zn^{2+} complexes predominantly present in solution and we achieved an in-depth molecular understanding of the spectral changes upon formation of the complex.

CPP 30.5 Wed 16:00 H 0107

Phase behavior and interactions of proteins in the presence of NaSCN — Mahnoush Madani[1], Nele Koch[1], Debes Ray[2], Jan K. G. Dhont[2], Kyongok Kang[2], and •Florian Platten[1,2] — [1]HHU Düsseldorf, Faculty of Mathematics and Natural Sciences, Düsseldorf, Germany — [2]FZ Jülich, IBI-4, Jülich, Germany

The state diagram of protein (lysozyme) solutions in the presence of sodium thiocyanate (NaSCN) is determined experimentally. Compared to NaCl, far lower salt concentrations are necessary to induce crystal formation and liquid-liquid phase separation (LLPS), respectively. These findings suggest a salt-specific effect of the SCN anion, strongly increasing net inter-protein attractions. Indeed, small-angle x-ray scattering experiments, used to determine the effective structure factor of the protein solutions, indicate a decrease of the second virial coefficient with SCN content, corresponding to increased net attractions.

15 min. break

CPP 30.6 Wed 16:30 H 0107

The effect of electric fields on the structure of water/acetonitrile mixtures — •Anastasios Sourpis, Nancy C. Forero-Martinez, and Friederike Schmid — Johannes Gutenberg University, Mainz

We study the effect of macroscopic electric fields on the structure of water/acetonitrile mixtures at high acetonitrile content by molecular dynamics simulations. We find that the linear response regime extends up to roughly 0.1 V/nm^{-1} in these mixtures, then nonlinear behavior sets in. The most pronounced nonlinear effect of an electric field is a change of relative orientations of neighboring acetonitrile molecules, from predominantly antiparallel to predominantly parallel. Nevertheless, the hydrogen bond network topology remains remarkably stable and conserves its overall properties in the whole range of considered applied fields up to 0.5 V/nm^-1, which is far beyond the dielectric breakdown limit of pure water. Additionally, we report on a comparison of simulation results at zero field with experimental results and available ab-initio data using four different recently proposed acetonitrile force fields, where we find that the force field by Kowsari and Tohidifar [J. Comput. Chemistry 39, 1843, 2018] performs best. Furthermore, we demonstrate that analyzing the hydrogen bond network can be a useful tool in investigating the formation and structure of water nanodomains and their confinement by an acetonitrile matrix in water/acetonitrile mixtures.

CPP 30.7 Wed 16:45 H 0107

Solvent Effects on Structure and Screening in Confined Electrolytes — •Henrik Stooss[1], Svyatoslav Kondrat[2,3], Christian Holm[2], and Alexander Schlaich[1,2] — [1]Stuttgart Center for Simulation Science (SC SimTech), University of Stuttgart, 70569 Stuttgart, Germany — [2]Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany — [3]Institute of Physical Chemistry, Polish Academy of Sciences, 01-224 Warsaw, Poland

The study of electrostatic interactions in room-temperature ionic liquids and concentrated electrolytes has gained significant attention due to recent findings indicating unexpectedly extensive screening lengths at high ion concentrations, termed underscreening. This phenomenon challenges classical theories, suggesting it arises from bulk properties but lacks prediction under experimental conditions. Despite extensive simulations and theoretical efforts, the origin of these long screening lengths remains elusive.

Here, we employ classical density functional theory (cDFT) and atomistic molecular simulations to study concentrated electrolytes. Using implicit and explicit solvent models, we analyse how solvent structure and its discrete nature influence short and long-range screening in concentrated ionic systems. Our cDFT reproduces ion adsorption at charged interfaces compared to our atomistic simulation approach that accounts for the solvent and ion exchange with a reservoir. Our work highlights the impact of solvent particles on screening mechanisms and provides insights into the intricate behaviour of electrostatic correlations in highly concentrated ionic environments.

CPP 30.8 Wed 17:00 H 0107

Ferroelectric Nematic Fibers: Nonlinear optical response and behaviour in electric fields. — •Alexander Jarosik, Hajnalka Nádasi, and Alexey Eremin — Otto-von-Guericke Universität, Magdeburg, Germany

The discovery of ferroelectric nematics (NFs) with vector symmetry has ushered in a novel area of liquid crystal research. Being the first true 3D ferroelectric fluid, NFs show a wide variety of electro-optical, electro-mechanical and nonlinear optical phenomena. Here, we demonstrate the formation of the slender freely suspended ferroelectric liquid fibers. We discuss their stability, thinning dynamics and electro-optical properties.

CPP 30.9 Wed 17:15 H 0107

From cellulose model surfaces to novel paper materials — •Cassia Lux, Leonie Beer, 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. The functionalization of paper with stimuli-responsive microgels enables the preparation of biosensors or paper with new mechanical properties, such as higher flexibility. In order to study the particle adsorption, planar cellulose model surfaces are prepared to mimic the surface of a cellulose fiber. The impact of the charge and crosslinker content of the positively charged PNIPAM microgels on the adsorption to the negatively charged cellulose surface is studied. The question we address is how the properties of the particles affect the contact area between both and what impact this has on the adhesion. The structure of the particles and the force required to move the particles are studied by (peak force) AFM.

CPP 30.10 Wed 17:30 H 0107

Equilibrium and resilience to external and internal influences of switchable windows based on metal electrodeposition — •Rebecca Cizek[1], Florian Sutter[1], Kai Gehrke[2], Eckhard Lüpfert[1], Stephan Heise[2], and Robert Pitz-Paal[1] — [1]DLR, Institut für Solarforschung, Almeria, Spain — [2]DLR, Institut für Vernetzte Energiesysteme, Oldenburg, Germany

To reduce the rising energy demand for climate control in buildings with large window area, switchable windows get increased attention. Such windows can be used on façades of buildings but also on greenhouses. Switchable windows can change their transmittance mostly though an electric stimulus (electrochromic). The investigated windows consist of an electrolyte sandwiched between two electrodes and covered by a closure. The transmittance changes when metal is deposited by applying a voltage (electrodepositon). This process can be reversed either by application of voltage in the opposite direction or over time (hours). The latter, called self-bleaching, is a counteracting process to the electrodeposition. The equilibrium between those processes corresponds to a balance between the deposition and the self-bleaching rate of the metal. We identified the equilibrium voltage and its resilience to several parameters, including internal parameters like composition and viscosity of the electrolyte and the material and surface roughness of the electrodes as well as external parameters like temperature and humidity. This allows optimizing the setup towards lower energy consumption and appropriate transmittance changes for greenhouse application.

CPP 30.11 Wed 17:45 H 0107

Pressure effect on protein cluster formation induced by multivalent ions — •Marcell Wolf[1], Christian Beck[2,3], Judith Peters[3], and Tilo Seydel[3] — [1]Heinz Maier-Leibnitz Zentrum, Technische Universität München, Germany — [2]Institut für Angewandte Physik, Universität Tübingen, Germany — [3]Institut Max von Laue - Paul Langevin (ILL), Grenoble, France

A thorough understanding of protein interactions in aqueous solutions is crucial for many areas of research in soft matter and biology. For example, a strong interprotein attraction can lead to protein aggregation, which is observed in several pathologies such as cataract and neurodegenerative diseases. We have shown that a patchy particle model can describe the phase behavior of a system of acidic globular proteins such as bovine serum albumin in the presence of multivalent salts such as yttrium chloride. The phase diagram of the studied system as a function of salt concentration and temperature is quite complex, showing reentrant condensation, metastable liquid-liquid phase separation, cluster formation and crystallization. In particular, a lower critical solution temperature is observed which suggests that hydration plays an essential role in the ion-mediated protein interactions. Here we will present results from pressure dependent neutron spectroscopy experiments. In contrast to the previous studies at and above room temperature we found, that the slowing down of the short-time self-diffusion is less pronounced. This behavior of the short-time self-diffusion will be discussed with the help of pressure dependant SAXS measurements.

CPP 31: Organic Electronics and Photovoltaics II

Time: Wednesday 15:00–17:45 Location: H 0110

CPP 31.1 Wed 15:00 H 0110

N-type charge transfer complex in DBTTF:HATCN mixtures — •Hongwon Kim[1], Andreas Opitz[2], Marie Siegert[3], Lennart Frohloff[2], Jens Pflaum[3], and Wolfgang Brütting[1] — [1]Experimental Physics IV, Institute of Physics, University of Augsburg, Germany — [2]Supramolecular System, Institute of Physics, Humboldt University of Berlin, Germany — [3]Experimental Physics VI, University of Würzburg, Germany

Mixtures of the electron donor DBTTF and the acceptor HATCN form a charge transfer complex (CTC), which leads to the appearance of new optical absorption bands below the band gap of the two pristine materials and a significant enhancement of the electrical conductivity. We prepared thin films by co-evaporation through systematic variation of their mixing ratio from pure DBTTF to pure HATCN and measured the temperature-dependent conductivity as well as charge carrier concentration and mobility. Surprisingly, we found n-type behavior for all compositions, except pure DBTTF. This can be understood from the electronic structure of the mixtures through ultraviolet photoelectron spectroscopy (UPS), which conclusively indicate that charge injection and transport occurs via the lowest unoccupied molecular orbital (LUMO) of the CTC. Furthermore, insight into the rich behavior of the electrical conductivity can be gained from morphological studies using Atomic Force Microscopy (AFM).

CPP 31.2 Wed 15:15 H 0110

Effective Electron-Vibration Coupling Constants by Ab Initio Methods — •Maximilian Franz-Xaver Dorfner and Frank Ortmann — TUM School of Natural Sciences, Technische Universität München, 85748 Garching b. München, Germany

This contribution is concerned with the analysis of different levels of theory for calculating the linear electron-phonon coupling constants. To bridge between density functional theory (DFT) and higher-level many-body approaches, we make use of the quasi-particle picture. Within this framework, we derive an effective quasi-particle linear coupling Hamiltonian, which describes the interaction of quasi-particles with phonons. We use this description to establish an approximate connection between the coupling constants calculated with DFT and higher-level many-body approaches by identifying the Kohn-Sham potential as an approximation to the static part of the self-energy. We determine the conditions under which a pragmatic DFT approach yields, in principle, the same coupling constants as a numerically much more expensive many-body approach. To test the theory, we finally compare the respective coupling constants for a few small molecules. The numerical results are found to be in good agreement with the presented theory.

CPP 31.3 Wed 15:30 H 0110

Organic photomultipliers working as reservoir — •Klara Hänisch, Hans Kleemann, Johannes Benduhn, and Karl Leo — TU Dresden, Dresden, Deutschland

Reservoir Computing (RC) is a well-known and often-used tool for classification, time prediction or recognition tasks. But software-based computing always has the disadvantage of a high power consumption, latency and the need to digitalize input data. How tempting is therefore the idea of reservoir computing directly implemented in hardware with a low power supply consumption and analogous data handling. Hardware-based RC is a promising concept for direct processing of analog inputs with drastically reduced training effort compared to conventional machine learning techniques. In this work we explore the application of organic photomultipliers as non-linear nodes for hardware-based RC. In particular, we investigate the origin of the nonlinearity, its wavelength-,and frequency-dependent response and discuss possible implication scenarios for reservoir computing. Furthermore, we show that the strength of the nonlinear coupling is connected to the external quantum efficiency of the cell, which opens up the possibility to discriminate selected spectral ranges.

CPP 31.4 Wed 15:45 H 0110

Understanding the Mechanism of Giant Surface Potential (GSP) in Evaporated Organic Thin Films: A Molecular Dynamics Simulation Approach — •Muhammad Nawaz Qaisrani[1], Naomi Kinaret[1], Felix Post[1], Falk May[2], and Denis Andrienko[1] — [1]Max Plank Institute for Polymer Research, Mainz, Germany — [2]Merck Electronics KGaA, Darmstadt, Germany

The emergence of the Giant Surface Potential (GSP) in evaporated organic thin films has gained considerable attention in recent years. However, the molecular mechanism underlying the spontaneous orientation of the net dipole moment that gives rise to GSP remains poorly understood. In this work, we employed coarse-grained molecular dynamics simulations to replicate vacuum deposition experiments and generate the morphology of evaporated thin films consisting of organic semiconductor materials. The simulated morphologies predicted well the orientation of molecular dipoles within the film, yielding the correct sign of the GSP. Notably, our simulation protocol incorporated electrostatic interactions in a coarse-grained model, which was crucial in accurately predicting the sign of experimental GSP. Our findings provide valuable insights into the molecular structure of these thin film materials and their applications in organic electronic devices.

CPP 31.5 Wed 16:00 H 0110

A novel organic ferroelectric with two parallel sublattices? — ●Ramon Jannasch[1], Maximilian Litterst[1], Manjunath Balagopalan[2], Elin Dypvik Sødahl[2], Ola Nilsen[2], Carl Henrik Gørbitz[2], Kristian Berland[2], and Martijn Kemerink[1] — [1]IMSEAM, Heidelberg University, Heidelberg — [2]Department of Chemistry, Norwegian University of Life Science, Oslo

Ferro- and piezoelectric materials find common usage in a range of electronic devices. Although inorganic materials so far dominate the field, they come with significant drawbacks, including energy-intensive production, reliance on toxic and/or rare elements and a lack of mechanical flexibility. Organic ferroelectric may offer a solution to some or even all of these problems.

Here, we investigate the organic material hexamethylenetetramine hydrogen DL-malate through various measurements aimed at assessing its ferroelectric behavior. Combining dielectric relaxation spectroscopy (DRS), capacitance-voltage (CV)-measurements and polarization hysteresis measurements using the double wave method (DWM), we obtain a comprehensive understanding of its ferroelectric properties. The observation of singularities in DRS, a butterfly loop in the CV-measurement, and a saturating switchable polarization during DWM collectively indicate bona fide ferroelectricity. At the same time, we find indications for the presence of two ferroelectric sublattices with different coercive fields but parallel alignment in the ground state.

15 min. break

CPP 31.6 Wed 16:30 H 0110

Charge transfer states do not like cold charges — ●Tobias Krebs, Clemens Göhler, and Martijn Kemerink — Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University

The power conversion efficiency of organic solar cells still lags behind their inorganic counterparts. Especially the open circuit voltage (Voc) losses are currently hard to reduce without knowing their exact origins. As different loss mechanisms have distinct temperature and light intensity dependencies, looking at Voc not only at room temperature and 1 sun illumination but also at lower and higher temperatures as well as at lower light intensities to pinpoint the dominant loss channel is imperative. We develop a new analytical rate-equation model based on previous work by Koster et al. [1], which allows us to distinguish different loss channels and incorporates the specific, far-from-equilibrium charge carrier dynamics in organics. For our PM6:Y6 solar cells, the model fits the experimental data over the range of applied temperatures down to 90K and light intensities as low as 1e-6 suns. Our results further suggest that the voltage losses at low light intensities and temperatures are mostly due to charges being stuck in the interfacial charge transfer state. Additionally, we benchmark the model against kinetic Monte Carlo simulations and find good agreement of Voc as well as recombination and escape yields.

[1] *Quantifying Bimolecular Recombination Losses in Organic Bulk Heterojunction Solar Cells*, Koster et al. Advanced Materials 23, 1670*1674 (2011).

CPP 31.7 Wed 16:45 H 0110

Identify the losses occurring in all-polymer solar cells — ●Shahidul Alam[1], Wejdan Althobaiti[1], Safakath Karuthedath[1,2], Ning Su[3], Christopher E. Petoukhoff[1], José P. Jurado[1], Oleksndr Matiash[1], Amr Dahman[1], Khawla Alkhezaim[1], Vladimir Dyakonov[4], Andreas Sperlich[4], Vojtech Nádaždy[5], Tobin J. Marks[3], Antonio Facchetti[3], and Frédéric Laquai[1] — [1]KAUST, Kingdom of Saudi Arabia — [2]Tsinghua University, Shenzhen, China — [3]Northwestern University, USA — [4]University of Wurzburg, Germany — [5]Slovak Academy of Sciences, Slovak Republic

For unknown reasons, small molecule non-fullerene acceptor-based bulk heterojunction OSCs are ahead of all-polymer solar cells. Here, blends of the donor polymers PCE12 and PM6 with two acceptor polymers, PYN-BDT and PYN-BDTF, are used to study PCE-limiting processes in solar cells. The π-extended naphthalene rings in these compounds make them macromolecular absorbers with large optical cross-sections up to 900 nm. Combining steady-state optical spectroscopy, TRPL, TA, ESR, and TDCF experiments provides a concise and quantitative assessment of losses due to limited photon absorption, geminate and non-geminate recombination (NGR), field-dependent charge generation, and inefficient carrier extraction. Pulsed-laser spectroscopy kinetic parameters reproduce experimentally measured device IV characteristics and show that low FFs are caused by NGR competing with charge extraction or a strong field dependence of charge generation, depending on the acceptor polymer.

CPP 31.8 Wed 17:00 H 0110

Loss mechanisms in low-bandgap organic solar cells — ●Guorui He[1], Atul Shukla[1], Yonglin Cao[2,6], Yufei Gong[3], Nurlan Tokmoldin[2], Bowen Sun[1], Drew Riley[4], Mohammad Shadabroo[2], Julian Steele[5], Ardalan Armin[4], Lei Meng[3], Yongfang Li[3], Safa Shoaee[2], Dieter Neher[1], and Felix Lang[1] — [1]Soft Matter Physics and Optoelectronics, University of Potsdam, Germany — [2]Disordered Semiconductor Optoelectronics, University of Potsdam, Germany — [3]Chinese Academy of Sciences, China — [4]Swansea University, United Kingdom — [5]The University of Queensland, Australia — [6]South China University of Technology, China

We investigate and compare the loss mechanisms of low-bandgap OSCs based on the blend of the donor polymer PTB7-Th with two different NFAs BTPV-4F-eC9 and BTPV-4Cl-eC9, with a bandgap of 1.24 eV and 1.26 eV, respectively. Both NFAs exhibit the same conjugated core, except that in BTPV-4Cl-eC9, the four terminal fluorine atoms are replaced by four chlorines.

To understand how the change of the terminal groups is affecting the device performance, we investigate the various recombination processes of the two systems. The results show that the PTB7-Th:BTPV-4Cl-eC9 blend suffers from stronger bimolecular recombination and geminate recombination. In addition, EMPL reveals a significant voltage loss in both blends. Temperature-dependent SCLC measurements show a rather low electron mobility in PTB7-Th:BTPV-4Cl-eC9 system, which we relate to a larger disorder of the LUMO.

CPP 31.9 Wed 17:15 H 0110

Enhanced air stability with solid additive EH-P in PBDB-TF-T1:BTP-4F-12 solar cells — ●Zerui Li[1], Sergei Vagin[2], Kun Sun[1], Xiongzhuo Jiang[1], Renjun Guo[1], Matthias Schwartzkopf[3], Stephan V. Roth[3,4], Bernhard Rieger[2], and Peter Müller- Buschbaum[1,5] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]TUM School of Natural Sciences, Wacker Chair of Macromolecular Chemistry, 85748 Garching, Germany — [3]DESY, 22607 Hamburg, Germany — [4]KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden — [5]MLZ, TUM, 85748 Garching, Germany

Additive plays an important role in organic solar cells. Traditional additives are most liquid, such as DIO, CN, DPE. Nowadays solid additives have called more research interest due to their various advantages in morphology-directing abilities, post treatment, enhanced device performance and stability. We explored an effective solid additive EH-P in green-solvent based organic solar cells (PBDB-TF-T1: BTP-4F-12). Greatly increased device performance and stability were achieved with EH-P doping. In-situ GIWAXS and GISAXS were used to observe the evolution of micro-structure and crystallinity during the degradation process in air under illumination. The stability increasement mainly comes from morphology modification rather than photo-oxidation, which was proved with charge mobility measurement and UV-vis spectrum.

CPP 31.10 Wed 17:30 H 0110

What makes thickness-tolerant organic solar cells? — Xabier Rodríguez-Martínez[1], ●Constantin Tormann[2], Marta Sanz[3,4], Bernhard Dörling[3], Martí Gibert-Roca[3], Albert Harillo-Baños[3], Enrique Pascual-San-José[3], José Piers Jurado[3], Laura López-Mir[4], Martijn Kemerink[2], and Mariano Campoy-Quiles[3] — [1]Institute for Physical Chemistry, Heidelberg University, Germany — [2]Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University, Germany — [3]Instituto de Ciencia de Materiales de Barcelona, Bellaterra, Spain — [4]EURECAT, Centre Tecnológic de Catalunya, Barcelona, Spain

Thick-film organic photovoltaics (>200 nm) are desirable to spark commercialization through mass-printing methods. Thickness resilient materials are, however, scarce and not fully understood. In this work, 17 different donor:acceptor blends are screened in terms of photoactive layer (PAL) thickness to build a consistent database of 649 inverted devices. The experimental results can be categorized into to two main blend families: one being resilient against increased PAL thickness whereas short-circuit current (JSC), fill factor (FF) and power conversion efficiency (PCE) decrease in the second family. Our kinetic Monte Carlo (kMC) simulations show how the blend morphology alone is able to explain the trends of both blend families without tweaking of recombination parameters (cf. drift-diffusion). The kMC simulations further predict the open-circuit voltage (VOC) to be uncorrelated to the PAL thickness which agrees with the experimentally observed trends for VOC in both blend families.

CPP 32: Focus Session: Novel Approaches to Surface Plasmon Generated Charges and Heat for Photocatalysis I (joint session O/CPP)

Plasmonic nanostructures present efficent optical antennas to generate energetic charges and/or localized heat for the use in photocatalysis. The time and length scales of typical plasmon-induced processes however pose a formidable challenge, which today still hinders the large-scale implementation of plasmon photocatalysis. The aim of this focus session is to discuss the physical mechanism of plasmon-induced charge-transfer and heat generation processes and exchange ideas on novel materials and devices utilizing these processes.

Organizers: Marc Herzog, Wouter Koopman (U Potsdam)

Time: Wednesday 15:00–17:30 Location: MA 141

Topical Talk CPP 32.1 Wed 15:00 MA 141

Plasmonic photothermal chemistry on single nanoparticles — •Andrea Baldi — Vrije Universiteit Amsterdam, The Netherlands

Metal nanoparticles strongly absorb light thanks to light-driven oscillations of their free electrons called plasmon resonances. The decay of these resonances can be used to drive chemical reactions via heating of the surrounding environment. In this talk, I will show how we quantify photothermal heating on single nanoparticles using a novel Raman-based thermometry [1] and how we use localized temperature gradients to drive the synthesis of hierarchical core-shell nanostructures [2].

[1] P. Li, S. H. C. Askes, E. del Pino Rosendo, F. Ariese, C. Ramanan, E. von Hauff, and A. Baldi, Nanoscale Thermometry of Plasmonic Structures via Raman Shifts in Copper Phthalocyanine, J. Phys. Chem. C 2023, 127, 9690-9698

[2] R. Kamarudheen, G. Kumari, and A. Baldi, Plasmon-driven synthesis of individual metal@semiconductor core@shell nanoparticles, Nature Communications 2020, 11:3957

CPP 32.2 Wed 15:30 MA 141

Single molecule layer temperature control via electrically connected SERS gratings — •Thorsten Feichtner[1], Pooja Sutheeshnan[2], Paul Mörk[1], Enno Schatz[3], and Bert Hecht[1] — [1]Nano- Optics & Biophotonics Group, Department of Experimental Physics 5, Röntgen Research Center for Complex Material Research (RCCM), Physics Institute, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]School of Physics, IISER Thiruvananthapuram, India — [3]NanoStruct GmbH, Friedrich-Bergius-Ring 15, 97076, Würzburg

It would be beneficial for photoelectrochemical experiments in microfluidic environments to be able to locally heat and directly measure the realized temperature. Surface enhanced Raman scattering can be used to locally measure the temperature of molecules, as the scattering peak heights depend on the probability density of vibrational states.

Here we provide evidence that our recently developed two wire grating SERS substrates [1] can be heated very locally using its Ohmic resistance. We measure its resulting temperature using the Raman peaks of a self-assembled monolayer of 4-MBA molecules in dependency of the heating current and fitting a probability density function approach. We back up the experiment with optical and heat simulations. This platform is ready to be implemented in microfluidic systems to measure SERS at the very same position where heat is applied.

[1] Sweedan, Amro, et al., arXiv preprint arXiv:2308.01395 (2023).

CPP 32.3 Wed 15:45 MA 141

Superlattice excitation driven by electron-phonon interaction measured with UXRD — •Jan-Etienne Pudell[1], Marc Herzog[2], Max Mattern[2], Alexander von Reppert[2], Daniel Schick[3], Ulrike Boesenberg[1], Angel Rodriguez-Fernandez[1], Wonhyuk Jo[1], Roman Shayduk[1], Wei Lu[1], Gregory Malinowski[5], Michel Hehn[5], Matias Bargheer[2,4], and Anders Madsen[1] — [1]European XFEL, Germany — [2]Institut für Physik, Uni Potsdam, Germany — [3]MBI, Berlin — [4]HZB Berlin, Germany — [5]IJL, Université Lorraine, France

The transport of heat (or energy in general) in nanoscopic heterostructures is of great fundamental as well as technological interest, e.g. in the context of thermal management in devices, heat-assisted magnetic recording or plasmonic catalysis. In metal heterostructures, heat conduction is usually dominated by electrons which can be at strong non-equilibrium with lattice vibrations on ultrashort time scales. Utilizing ultrafast x-ray diffraction (UXRD) at the MID end-station at European XFEL, we investigate the ultrafast structural response of a laser-excited metal-metal superlattice (SL) consisting of few-nm thick metal layers with low (Cu) and high (Pt) electron-phonon coupling on top of a 100 nm Cu and 20 nm Ni layer. Using the transient shift and intensity modulations of the respective Bragg peaks, we can quantify the ultrafast heat flow in the SL by comparison to a time-dependent diffusive two-temperature transport model. We identify the excitation of the SL phonon mode as well as an efficient heat transport from the laser excited SL to the Ni-layer via hot electrons.

CPP 32.4 Wed 16:00 MA 141

How to evaluate temperature at single-molecule, single-particle and ensemble levels — •Simone Ezendam, Julian Gargiulo, and Emiliano Cortés — Physics department, University of Munich, Germany

Understanding temperature dynamics across various scales (single-molecule, single-particle, and ensemble) is pivotal in harnessing plasmonic catalysis for enhanced chemical reactivity. We present three studies investigating this intricate interplay. First, employing super-resolution fluorescence microscopy, we probe single-particle plasmonic catalysis, unveiling distinct pathways and spatial reactivity [1]. Second, through single-particle thermometry, we explore morphology-driven light-to-heat conversion in Au/Pd nanoparticles, unraveling intriguing photothermal responses [2]. Finally, we introduce Anti Stokes thermometry to measure temperature in plasmonic ensembles, validating its efficacy in understanding light-induced heating of nanoparticle arrays [3]. These findings deepen our understanding of plasmonic heating, guiding the design of future nanocatalysts.

[1] 10.1021/acsnano.3c07833, [2] 10.1038/s41467-023-38982-9 [3] 10.1002/adom.202301496

CPP 32.5 Wed 16:15 MA 141

Measurement of temperature gradients at plasmonic metal surface using thermosensitive microgels — •Yulia Gordievskaya[1], Nino Lomadze[1], Se-Hyeong Jung[2], Andrij Pich[2,3], and Svetlana Santer[1] — [1]University of Potsdam, Potsdam, Germany — [2]RWTH Aachen University, Aachen, Germany — [3]Aachen Maastricht Institute for Biobased Materials (AMIBM), Geleen, The Netherlands

Microgels are recognized for their remarkable responsiveness to changes in environmental conditions[1]. Here, we presented a novel method for local temperature determination in aqueous solutions by observing the inhomogeneous collapse of microgels positioned at plasmonic metal surface. The surface is a variable-thickness gold layer(5-30nm) deposited on glass coated with titanium oxide(<1nm). The localized laser irradiation of the substrate results in the absorption of light by the gold layer, converting it into heat [2]. We studied how the laser wavelength and power levels, as well as distance from the irradiation spot influence the size and shape of the thermosensitive PNIPAM microgel. The obtained dependences allowed us to construct a comprehensive temperature distribution profile relative to the irradiation point.

We thank SFB 1636: Elementary processes of light driven reactions at the nanoscale. [1] J. Jelken, S.-H. Jung, N. Lomadze, Yu.D. Gordievskaya, E.Yu. Kramarenko, A. Pich, S. Santer. Advanced Functional Materials 32.2 (2022), p. 2107946. [2] V. Muraveva, M. Bekir, N. Lomadze, R. Großmann, C. Beta, S.Santer. Applied Physics Letters 120.23 (2022), p. 231905.

Topical Talk CPP 32.6 Wed 16:30 MA 141

Disentangling plasmonic catalysis contributions by time-resolved spectroscopy — •Holger Lange — The Hamburg Centre for Ultrafast Imaging — Institute of Physics and Astronomy, University of Potsdam

According to current understanding, the nanoparticle plasmon decay is a series of sequential scattering events, separated by their timescales of vastly increasing duration. At first, Landau damping polarizes the electron density. Electron-electron scattering equilibrates the excess energy and subsequent electron-phonon coupling leads to rapid electron cooling and a simultaneous increase in lattice temperature. Several of these processes might contribute to the reaction rate enhancement on plasmonic nanoparticles. I will discuss a range of experiments to specifically address the individual steps of the plasmon decay. The temperature of the thermalized hot electron gas can be observed as a contrast in optical pump-probe experiments, the excited lattice is accessible by time-resolved x-ray scattering. I will present the first reconstruction of the decaying gold nanoparticle plasmon field in the time domain by the detection of transient currents. This data combined with reaction dynamics studies under monochromatic excitation reveals both, non-equilibrium carriers and field-induced excitation as most relevant contributions for two different reactions, highlighting the selectivity of the processes.

CPP 32.7 Wed 17:00 MA 141

In situ Observation of Nanoparticle Photocharging: Gold Nanorods as Photochemical Capacitors — •Felix Stete[1], Wouter Koopman[1], and Matias Bargheer[1,2] — [1]Institut für Physik & Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [2]Helmholtz Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany

Light can induce charge on plasmonic nanoparticles. This idea was used in the last years to explain experimental results on chemical reactions on gold and silver nanoparticles. Here, we give spectroscopic evidence for this photocharging effect and present a method to examine the charge transfer from a hole scavenger to gold nanorods in situ. In contrast to the plasmon resonance in gold nanospheres, the longitudinal resonance of gold nanorods is very sensitive to the free electron density in the metal. We show here how the illumination with light blue-shifts the resonance visualizing the transfer of electrons from ethanol in the solution to the nanoparticles and model the intensity-dependence in a capacitor model. The peak can also be shifted back again after illumination when the particles are left in dark or exposed to molecules with a low reduction potential. We discuss how particle size, oxygen in the solution or the absence of ethanol influence the particle charging.

CPP 32.8 Wed 17:15 MA 141

Catalytic Electron Transfer Inhibited by Coulomb Blockade in Au Nanoparticles — •Monalisa Garai and Thomas Klar — Institute of Applied Physics, Johannes Kepler University Linz, Altenberger Straße 69, 4040 Linz

Colloidal noble metal nanoparticles (NPs) are excellent catalysts for various chemical redox reactions. They offer alternative reaction pathways and thereby significantly reduce the activation energy for chemical transformations. There are several strategies to reduce the activation energy for kinetically sluggish catalytic reactions, e.g. by changing the size, shape and composition of the NPs and also by changing the specific reaction conditions. To investigate the reaction mechanism of Au NPs of different sizes below 10 nm, we used the 1-electron transfer from ferricyanide (Fe3+) to ferrocyanide (Fe2+) as a model reaction system. We compared the reaction rate of the conversion from Fe3+ to Fe2+ in the presence and absence of the reducing agent triethanolamine (TEOA). It has been shown that the reaction pathway is significantly altered with and without TEOA. TEOA generally transfers electrons to Au NP and causes a negative charging on the Au NP surface. However, if the size of the NPs is very small, especially below 5 nm, the negative charging of the Au NPs is inhibited by the Coulomb blockade effect. As a result, the subsequent catalytic electron transfer from Au NP to Fe3+ is also inhibited, which decreases the overall Fe3+ reduction rate. These experimental results and theoretical calculations will help to develop novel metal NPs for various catalytic processes for environmental remediation.

CPP 33: Hybrid and Perovskite Photovoltaics I

Time: Wednesday 16:30–18:00 Location: H 0106

CPP 33.1 Wed 16:30 H 0106

Structure and morphology investigations on printed perovskite quantum dot films — •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, 85748 Garching — [2]Nano-Institut München und Fakultät für Physik, LMU, 80539 München — [3]Department Chemie und CeNS, LMU, 81377 München — [4]DESY, 22607 Hamburg — [5]MLZ, TUM, 85748 Garching

Solar cells based on thin-film architectures offer potentially cheaper production, semi-transparency, and flexibility. Slot-die coating is one of the most promising scalable and roll-to-roll compatible deposition method for thin-film solar cells. Printing thin-film layers from colloidal quantum dot solution offers the advantage of decoupling the crystallization from the deposition process. Perovskite quantum dots are one option for high-quality next-generation perovskite solar cells. We demonstrate the feasibility of fabricating solar cells from printed quantum dots as the active layer. Extensive characterization by SEM and grazing-incidence X-ray scattering gives insights into the morphology, structure, and texture. SEM, FLIM, PL, and transient PL measurements shed light on the optoelectronic properties of the solar cell printed from colloidal hybrid perovskite quantum dot solution.

CPP 33.2 Wed 16:45 H 0106

Time-resolved structure formation in perovskite thin films and powders — •Christopher Greve[1], Konstantin Schötz[2], Philipp Ramming[2], Fabian Panzer[2], Anna Köhler[2], Helen Grüninger[3], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group — [2]Lehrstuhl für Optoelektronik weicher Materie — [3]Inorganische Chemie III - all Universität Bayreuth, 95440 Bayreuth

To shift from a trial-and-error optimization methodology to a more systematic approach in optimizing metal halide perovskite (MHP) processing, it is imperative to enhance the understanding of MHP formation and the subsequent dynamical processes. To improve the understanding of thin film formation from solution we can utilize in situ PL, light scattering and absorption measurements to track the crystallization processes.[1] However, subsequent dynamic processes within the final MHP film also play a major role, as they define material stability. One example is phase segregation in mixed halide MHP, which we can track with in-situ XRD measurements at various temperatures.[2] Another tool to study dynamics in MHP films is grazing incidence X-ray correlation spectroscopy, which bulk-sensitive application to films results in altered correlation functions. We present an approach within the sDWBA to identify suitable measurement parameters for the application to MHP thin films.[3] [1]: Schötz, Greve et al., 10.1002/adom.202101161; [2] Greve, Ramming et al., 10.1021/acsenergylett.3c01878; [3]: Greve et al., 10.1021/acs.langmuir.3c00669

CPP 33.3 Wed 17:00 H 0106

Simulation of the Impact of Processing Conditions on the Perovskite Film Morphology — •Martin Majewski[1], Shudi Qui[2], Olivier Ronsin[1], Larry Lüer[2], Tian Du[2], Hans-J. Egelhaaf[2], and Jens Harting[1] — [1]Forschungszentrum Juelich GmbH, Helmholtz Institute Erlangen- Nuernberg (IEK-11), Dynamics of Complex Fluids and Interfaces, Cauerstraße 1, 91058 Erlangen, Germany — [2]Department of Materials Science and Engineering, Friedrich-Alexander-Universitaet Erlangen-Nuernberg, 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 present phase field simulations which are capable to describe the main physical processes: evaporation, diffusion, spontaneous nucleation, crystal growth and advection. The evaporation rate is modified in the experiment (by gas quenching) and simulation. The simulation is successfully validated against the experiments. With help of the simulation, the formation pathways for all investigated evaporation rates are uncovered. The ratio between evaporation and crystallization rate is identified as the main driver for the morphological transition from pinhole prone to pinhole free perovskite thin films.

CPP 33.4 Wed 17:15 H 0106

Deciphering the interplay of structure and charge carrier dynamics in reduced-dimensional perovskites — •Kun Sun[1], Renjun Guo[1], Shangpu Liu[2], Xiongzhuo Jiang[1], Yuxin Liang[1], Matthias Schwarzkopf[3], Felix Deschler[2], and Peter Müller-Buschbaum[1,4] — [1]TUM, TUM School of Natural Sciences, E13, Garching, Germany — [2]UOH, Physikalisch-Chemisches Institut, Heidelberg, Germany — [3]Desy, Hamburg, Germany — [4]TUM, MLZ, Garching, Germany

RDPs have advanced the development of PSCs due to their tunable energy landscape, structure, and orientation. Thus, we aim for an increase in the understanding of structure-photophysical properties of DJ and RP RDPs with different dimensionalities. Our findings reveal that RP RDPs with lower dimensionality exhibits a dominant n=2 phase, preferential out-of-plane orientation, and longer charge carrier lifetime compared with DJ RDPs, as evidenced by X-ray scattering technique and transient absorption spectroscopy. In addition, we unveil the film growth of respective RDPs by in-situ X-ray scattering, showing the stoichiometry-determined phase growth. The formation of lower-n phases in RP RDPs with higher dimensionality is thermodynamically favored, while those phases are likely in the form of intermediate phase, which bridge the 3d-like and lower-n phases in DJ RDPs. DJ RDPs with higher dimensionality demonstrate comparable phase purity, giving rise to more sufficient energy transfer and longer charge carrier lifetime. Our work paves the way for dictating the utilization of RDPs in both 3D and quasi-2D PSCs.

CPP 33.5 Wed 17:30 H 0106

Local Charge Carrier Dynamics in Lead Halide Perovskites by Nano Surface Photovoltage Spectroscopy — Yenal Yalcinkaya[1], Pascal Rohrbeck[1], Lukas Schmidt-Mende[2], and •Stefan A.L. Weber[1,3] — [1]MPI for Polymer Research, Mainz — [2]Department of Physics, University of Konstanz — [3]Institute for Photovoltaics, University of Stuttgart

Understanding electron and ion dynamics is an important task for improving lead halide perovskites based solar cells and related devices. Perovskite materials have a delicate nano- and micro structure that influences the device parameters. This study investigates the spatial defect distribution in the vicinity of grain boundaries (GB). To this end, we introduce Nano surface photovoltage spectroscopy (Nano-SPV) via time-resolved Kelvin probe force microscopy (tr-KPFM) [1,2]. By measuring the SPV decay on perovskite samples with small, large, and passivated grains, areas of increased charge carrier recombination, ion migration, and defects were locally detected [3]. Our results clearly show an improved uniformity of SPV and SPV decay distribution within the perovskite films upon passivation. Furthermore, the perovskite films with large grains show better recombination properties based on SPV decay and ideality factor values.

[1] Axt et al. Beilstein J. Nanotechnol. 9, 1809 (2018). [2] Weber et al., Energy Environ. Sci. 11, 2404 (2018). [3] Yalcinkaya et al. Adv. Opt. Mater. 2301318 (2023).

CPP 33.6 Wed 17:45 H 0106

CTAB assisted solvent-free mechanosynthesis of MAPbX3 nanocrystals: Stability, and photoresponse — •Gaurav Nim[1], Parul Bansal[2], and Prasenjit Kar[2] — [1]Department of Physics and Material Sciences Center, Philipps-Universität Marburg, Germany — [2]Department of Chemistry, Indian Institute of Technology Roorkee, India

In this work, hybrid metal halide perovskite, or HPs (MAPbX3, X = Br, I), was produced exclusively using multifunctional cetyl trimethylammonium bromide (CTAB) and the mechano-synthesis technique.* Equimolar amounts of MAX and PbX2 combined with a mmol quantity of CTAB were used to synthesize HPs. We did steady-state photoluminescence, X-ray diffraction (XRD), and time-correlated single-photon count (TCSPC) to look at the optical and structural properties of perovskite. The thermogravimetric analysis informs us about the thermal stability of the nanocrystals. X-ray diffraction analysis reveals that mechanochemically synthesized HPs show high crystallinity and phase purity, with stability over a period of time. The photoinduced current response of the perovskite reveals an excellent increase in photoconductivity when exposed to light (with a 1 V bias). The device fabricated of perovskite witnessed prompt photoresponse under light illumination and temporally stable photocurrent over multiple cycles of light irradiation. Due to their phase purity, low bandgap, nanoscale size, long-term stability, and easy-to-synthesis approach, the synthesized materials are useful for photovoltaic applications.

CPP 34: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods I

Time: Thursday 9:30–13:00 Location: H 0106

Invited Talk CPP 34.1 Thu 9:30 H 0106

Towards AI-assisted analysis of surface and small-angle x-ray and neutron scattering data — •Marina Ganeva — JCNS, Forschungszentrum Jülich, Jülich, Germany

The long term and sustainable success of Neutron and X-ray community essentially depends on its ability to meet growing challenges in handling and analyzing data of increasing volume and complexity. The arise of new generation of high-intensity x-ray and neutron sources and fast, large area 2D-detectors leads to high data rates and large data volumes, which are not possible anymore to analyze in traditional way. Thus, new fast and reliable approaches are required.

Nowadays AI-assisted approaches are increasingly being developed and applied to address the challenges in our life. They provide a smart solution with potential to accelerate the x-ray and neutron data analysis and facilitate the extraction of valuable insights from large and complex datasets. In the present talk I will discuss challenges and perspectives of AI-assisted data analysis for surface and small-angle x-ray and neutron scattering from soft matter samples and will give an overview of our recent results.

CPP 34.2 Thu 10:00 H 0106

Deep learning based reflectometry data analysis including prior knowledge — •Alexander Hinderhofer, Valentin Munteanu, Vladimir Starostin, Linus Pithan, Alexander Gerlach, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Current machine-learning solutions for automatized analysis of X-ray (XRR) and neutron reflectivity (NR) data is constrained by the range and number of considered parameters, making the approach inflexible for applying it to different material and layer configurations. To overcome this, we present an approach that utilizes prior knowledge to regularize the training process over larger parameter spaces. We demonstrate the effectiveness of our method in various scenarios, including multilayer structures with box model parametrization and a physics-inspired special parametrization of the scattering length density profile for a multilayer structure. In contrast to previous methods, our approach scales favorably when increasing the complexity of the inverse problem, working properly even for a several layer multilayer model and an N-layer periodic multilayer model with up to 20 open parameters. We will also discuss autonomous experiments enabled by machine-learning-based online data analysis in synchrotron beamline environments. [1]

[1] L. Pithan et al. J. Synchrotron Rad. 30 (2023) 1064

CPP 34.3 Thu 10:15 H 0106

Deciphering Electron Paramagnetic Resonance Spectra via Machine Learning — Shengchun Wang[1], Shufei Zhang[2], JIhu Su[5], •Yi Luo[3], and Aiwen Lei[4] — [1]Department of Medicinal Chemistry, University of Michigan, Ann Arbor, MI, USA — [2]Shanghai Artificial Intelligence Laboratory, Shanghai, China — [3]Institute of Functional Interfaces, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [4]College of Chemistry and Molecular Sciences, the Institute for Advanced Studies, Wuhan University, Wuhan , China — [5]Department of Modern Physics, University of Science and Technology of China, Hefei, China

Elucidating the properties of spin species is one of central issues in modern chemistry, material and biology science. For understanding these species, the rapid identification of isotropic and anisotropic Electron Paramagnetic Resonance (EPR) spectra is foundational. Conventional simulation methods, though detailed, often lag in efficiency. Here we present a hybrid approach integrating conventional computational method and Multi-Layer Perceptron (MLP) algorithms, leverages an extensive literature-derived EPR database, ensuring both speed and accuracy in species identification from EPR spectra. Evaluations validate its superior efficacy, attributing much to its robust database integration. This tool offers a promising bridge between academic rigor, computational efficiency, and EPR literature.

CPP 34.4 Thu 10:30 H 0106

JuMPO: A Quantum Optimal Control Library for Robust and Selective Magnetic Resonance Experiments — •Armin J. Römer[1,2], Simone S. Köcher[1], and Josef Granwehr[1,2] — [1]Forschungszentrum Jülich GmbH, IEK-9 — [2]RWTH Aachen University

Quantum optimal control is a versatile, powerful method to tailor magnetic resonance experiments both in terms of robustness and selectivity. Nevertheless, the method is not routinely employed in applied science. In order to make the engineering of such experiments more accessible, we have developed a quantum optimal control package adjusted to the language and needs of magnetic resonance spectroscopists. The package, Jülich Magnetic Pulse Optimization (JuMPO), offers a handy toolbox for both robust and highly selective magnetic resonance experiments. It enables optimizing for a range of Larmor frequency offsets and B_1 inhomogeneities, as well as the engineering of pattern pulses, where for each combination of offset and inhomogeneity a separate target state can be specified. Appropriate penalties can guide optimizations towards experimentally implementable pulse shapes. Furthermore, tools for chemically intuitive spin state preparation and spectrometer calibration parameters are featured. As a use case example, we present a set of robust broadband excitation and inversion pulses re-optimized with tighter robustness constraints than with previous pulse sequences. JuMPO can help to devise new, innovative experiments, which provide additional and more detailed information into complex systems, e.g. in catalysis or material science.

CPP 34.5 Thu 10:45 H 0106

Laser Diffraction for Defectoscopy of Cellulose Filaments — •Damien Pierce, Korneliya Gordeyeva, Anastasia Riazanova, Tomas Rosén, and Daniel Söderberg — KTH Royal Institute of Technology, Stockholm, Sweden

Filaments produced from the wet spinning of Cellulose nanofibrils are a promising alternative to those derived from fossil fuels. These filaments are the strongest bio-based filaments currently available, with potential uses in the production of high-performance textiles. However, establishing what the weakest point of such filaments is, has yet to be conclusively determined. We demonstrate the potential of laser diffraction as a defectoscopy technique. Tomograms of the apparent width of the filament were measured using laser diffraction and compared with SEM measurements. Tensile testing was performed in order to correlate the observed structures with the breakage point. We expect this technique to provide a rapid, non-destructive method of quality control, greatly speeding up the optimisation of processing conditions.

CPP 34.6 Thu 11:00 H 0106

Hydration layer ordering effects at gold - electrolyte interfaces confined by an atomic force microscope tip — •Martin Munz[1,2], Wiebke Frandsen[2], Beatriz Roldan Cuenya[2], and Christopher Kley[1,2] — [1]Helmholtz Young Investigator Group Nanoscale Operando CO2 Photo-Electrocatalysis, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany — [2]Department of Interface Science, Fritz Haber Institute of the Max Planck Society, 14195 Berlin, Germany

We introduce a correlative microscopy approach, combining in situ conductive atomic force microscopy (c-AFM) with simultaneous friction force and morphology imaging, thus enabling nanoscale physical-chemical interrogation of the catalyst - electrode interface. For the class of bimetallic electrocatalysts, the electric conductivity variations across nanopatterned CuOx islands on Au electrodes can be resolved in air, water and potassium bicarbonate aqueous electrolytes. In line with current contrasts between catalyst surface areas of different composition and oxidation state, I-V curves showed highly resistive CuOx islands. Simultaneously measured friction force images suggested a qualitative contrast variation upon transitioning from water to bicarbonate electrolyte, thus indicating that friction forces respond to hydration layer ordering effects. Complementary in situ AFM friction force measurements, using cantilevers with a high force sensitivity, revealed a decrease in the friction coefficient with increasing ionic concentration, for the low-concentration regime of a potassium perchlorate aqueous electrolyte, thus suggesting a chaotropic effect.

15 min. break

CPP 34.7 Thu 11:30 H 0106

Using Neural Network Potentials to Predict Thermal Iso-

merization Barriers for Spiropyran Derivatives — •Robert Strothmann[1], Johannes T Margraf[1,2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Universität Bayreuth, Bayreuth

First principles methods like density-functional theory can be used to study reaction barriers and give insights into the influence of chemical modifications on barrier heights and mechanisms. However, their large computational cost hinders their usage in high-throughput settings, which prevents large scale studies including thousands of structures. Surrogate models with reduced costs are therefore of great interest. In this context, neural network potentials (NNPs) have attracted much attention, as their uncertainty can be systematically decreased by increasing the amount and quality of the training data.

In this talk, we will highlight the usage of NNPs to assist in the prediction of thermal isomerization barriers of spiropyran photoswitches. This barrier governs the half-life of the thermal back-reaction, which is one of the key properties in photoswitch design. By utilizing transferability, NNPs trained on only a few spiropyran molecules and fine tuned in active-learning cycles allow the prediction of isomerization barriers for thousands of chemically modified spiropyrans. This not only gives a ranking of suitable photoswitches for a specific application, but also enables a more systematic study on how to tune the thermal half-life via chemical modification.

CPP 34.8 Thu 11:45 H 0106

Dedoping of PEDOT:PSS using Amines to shift the Threshold Voltage in OECTs — •Laura Teuerle, 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 34.9 Thu 12:00 H 0106

On Electron-Photon Correlation in Molecular Cavity QED with Low-Frequency Fields — •Eric W. Fischer[1] and Peter Saalfrank[2] — [1]Humboldt-Universität zu Berlin, Institut für Chemie, Brook-Taylor-Straße 2, 12489 Berlin — [2]Universität Potsdam, Institut für Chemie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam

Strong light-matter interaction of molecular systems with quantized field modes of optical micro-resonators form the building block of the rapidly evolving field of polaritonic chemistry.[1] In this contribution, we discuss the role of correlations between electrons and low-frequency cavity fields in molecular cavity QED from a quantum chemical perspective. We show that commonly employed effective ground state models further approximate the cavity Born-Oppenheimer (CBO) framework[2] by neglecting electron-photon correlation.[3] As connection, we introduce a CBO perturbation theory (CBO-PT), which is motivated by distinct electronic and IR cavity excitation energy scales.[3] Illustratively, we discuss the relevance of correlation corrections for reactive systems from the perspective of CBO-PT. Eventually, we show how to address vibro-polaritonic transmission spectra by combining CBO-PT with linear response theory.[4]

[1] T. W. Ebbesen, Acc. Chem. Res. 49, 2403 (2016).

[2] J. Flick et al., J. Chem. Theory Comput. 13, 1616 (2017).

[3] E.W. Fischer, P. Saalfrank, J. Chem. Theory Comput. 19, 7215, (2023).

[4] E.W. Fischer, J.A. Syska, P. Saalfrank, in preparation.

CPP 34.10 Thu 12:15 H 0106

Thermal expansion on molecular scale: heterogeneity and packing — •Martin Tress[1], Jan Gabriel[2], and Friedrich Kremer[1] — [1]Universität Leipzig — [2]Roskilde University, Denmark

While typically used for chemical characterization, infrared spectroscopy also reveals physical properties on molecular scale which are difficult to access otherwise. We study the thermal expansion of molecular bonds in amorphous systems, i.e. a series of polyalcohols as well as liquid water. By analyzing specific molecular vibrations and correlating them with interatomic bond lengths, the thermal expansion of covalent bonds and intermolecular hydrogen(H)-bonds is quantified. Pronounced differences between intra- and intermolecular expansion verify the dominance of the latter. Surprisingly, in polyalcohols the macroscopic thermal expansion (i.e. the cube root of inverse density) is even bigger than that of the strong H-bonds. This suggests that additional weak H-bonds or van-der-Waals contacts dominate the thermal expansion. Since strong H-bonds are the largest barriers to molecular rotation, i.e. they control the structural relaxation time, a clear explanation for the failure of density scaling - an attempt to link structural relaxation time with density - in H-bonding liquids is revealed. Liquid water exhibits an even more complex connection of intermolecular bond expansion and macroscopic expansivity due to the anomalous temperature dependence of its density. Our results demonstrate that heterogeneities in intermolecular contacts play distinct roles in densification and structural relaxation which requires explicit consideration in comprehensive theoretical descriptions of liquids and glass formers.

CPP 34.11 Thu 12:30 H 0106

A contribution from first principles to understand ageing mechanisms in polyethylene — •Guido Roma[1], Yunho Ahn[2], Yvette Ngono[3], and Muriel Ferry[4] — [1]Université Paris-Saclay, CEA, S2CM/SRMP, France — [2]Ewha Womans University, Photophysics Photochemistry Park Lab, Seoul, South Korea — [3]Normandie Univ., CEA, CIMAP Caen, France — [4]Université Paris-Saclay, CEA, SPC, France

The kinetics of radio-oxydation in polymers is still not yet fully elucidated, and polyethylene is a prototypical and important polymer material. In this paper we first developed an interface model in order to try to grasp the main atomic scale features of crystalline and amorphous regions; then we show how first principles calculations can be used to check the reliability of some kinetics schemes proposed in the literature. In particular, calculated energy barriers suggest that bimolecular reactions involving alkoxy radicals cannot be overlooked [1]. We also discuss of the mechanisms by which phenolic antioxidants are effective in delaying radio-oxidation in polyethylene. Finally, we show how the prediction of infrared spectra can be a valuable support for experimental investigation of the accumulated carbonyl concentrations through infrared spectroscopy [2].

Bibliography

[1] Y. Ahn, G. Roma, X. Colin, Macromol. **55**, 8676 (2022). [2] M. Ferry, Y. Ahn, F. Le Dantec, Y. Ngono, G. Roma, Polymers **15**, 1537 (2023).

CPP 34.12 Thu 12:45 H 0106

Near-surface free volume in polymers characterized by positron annihilation lifetime spectroscopy — •Christoph Hugenschmidt[1], Maik Butterling[2], Vassily Vadimovitch Burwitz[1], Adrian Langrehr[1], Lucian Mathes[1], Eric Hirschmann[2], Oskar Liedke[2], and Andreas Wagner[2] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Lichtenbergstr. 1, 85748 Garching, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics, 01328 Dresden, Germany

Positron annihilation lifetime spectroscopy (PALS) is a powerful technique for characterizing the free volume in polymers. The main drawback of conventional PALS, however, is the presence of a so-called source component due to positrons annihilating in the radioactive source material. By using a pulsed monoenergetic positron beam, as provided by MePS at the HZDR, the variable positron energy allows the depth-resolved PALS and the spectra intrinsically do not contain a source component. In order to investigate the mean pore size in various polymers, we recorded PALS spectra for positron implantation energies between 0.5 and 10 keV. The measured so-called pick-off lifetime of ortho-positronium allowed us to unambiguously determine the mean void size in the bulk. By analyzing the recorded PALS depth profiles changes of the free volume in the near-surface region of, e.g. polypropylene and polycarbonate could be observed.

CPP 35: Focus Session: Wetting on Adaptive Substrates I (joint session CPP/DY/O)

The focus session aims to discuss recent developments in the wetting dynamics of adaptive, deformable, and switchable surfaces.

Time: Thursday 9:30–11:00 Location: H 0107

Invited Talk CPP 35.1 Thu 9:30 H 0107

Extraordinarily slippery liquid-repellent surfaces using self-assembled monolayers — •Robin Ras — Aalto University, Espoo, Finland

Water-repellent surfaces have the attractive property of staying dry, and find applications in self-cleaning, anti-icing, anti-fogging and much more. Liquid-repellent surfaces, especially smooth solid surfaces with covalently grafted flexible brushes or alkyl monolayers, are the focus of an expanding research area.[1] Surface-tethered flexible species are highly mobile at room temperature, giving solid surfaces a unique liquid-like quality and unprecedented dynamical repellency.

We challenge two common assumptions on liquid-repellency.[2] It is generally assumed that water-repellent surfaces requires hydrophobicity. We demonstrate a hydrophilic surface with the unusual combination of low sliding angle and low contact angle. Surface heterogeneity is generally acknowledged as the major cause of increased contact angle hysteresis and friction of droplets. Here we challenge this long-standing premise for chemical heterogeneity at the molecular length scale.

Furthermore, we demonstrate world's most slippery surface, by combining self-assembled monolayers and surface structuring. Finally, by a suitable surface texture, we can trap a thin air layer for months, opening new strategies for underwater applications.[3]

[1] Nature Chemistry Reviews (2023) https://doi.org/10.1038/s41570-022-00455-w[2] Nature Chemistry (2023) https://doi.org/10.1038/s41557-023-01346-3 [3] Nature Materials (2023) https://doi.org/10.1038/s41563-023-01670-6

CPP 35.2 Thu 10:00 H 0107

Volatile binary mixtures on polymer brushes — •Jan Diekmann und Uwe Thiele — Institut für Theoretische Physik, Universität Münster, 48149 Münster, Germany

We present a mesoscopic thin-film model in gradient dynamics form for binary liquid mixtures on brush-covered substrates incorporating volatility in a narrow gap. Thereby, we expand models established in [1, 4-6] by incorporating two substances present in each of three bulk phases - liquid, brush and gas. We discuss the different contributions to the free energy, thereby employing Flory-Huggins theory of mixing for the condensed phases and assuming ideal gases for the vapor phase. Interface energies are modeled as linear interpolations of known limiting cases. The resulting six-field model is then analyzed with numerical time simulations showing results with a focus on lateral concentration gradients, notably at the contact line.

[1] S. Hartmann, C. Diddens, M. Jalaal, and U. Thiele. JFM 960, 2023. doi: 10.1017/jfm.2023.176. [2] S. Hartmann, J. Diekmann, D. Greve, and U. Thiele. 2023. doi: 10.48550/ARXIV.2311.07307. [3] S. Schubotz, Q. A. Besford, S. Nazari, P. Uhlmann, E. Bittrich, J.-U. Sommer, and G. K. Auernhammer. Langmuir, 39, 2023. doi: 10.1021/acs.langmuir.2c03009. [4] L. A. Smook, G. C. R. van Eck, and S. de Beer. Macromolecules, 53, 2020. doi: 10.1021/acs.macromol.0c02228. [5] U. Thiele and S. Hartmann. EPJ-ST 229, 2020. doi:10.1140/epjst/e2020-900231-2. [6] Özlem Kap, S. Hartmann, H. Hoek, S. de Beer, I. Siretanu, U. Thiele, and F. Mugele. JFM 158, 2023. doi: 10.1063/5.0146779.

CPP 35.3 Thu 10:15 H 0107

Wetting Phenomena in Hierarchically Porous Silicon: How Experiments and 2D Fluid-Dynamic Simulations Complement Each Other — •Stella Gries[1,2], Stefan Schulz[1], Marc Thelen[1,2], Silja Flenner[3], Imke Greving[3], and Patrick Huber[1,2] — [1]Institute for Materials and X-ray Physics, Hamburg University of Technology, Hamburg, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [3]Institute of Materials Physics, Helmholtz Zentrum Hereon, Geesthacht, Germany

Nature is an expert in designing highly efficient, multi-functional (hybride-)materials such as hierarchically capillary systems in respiratory systems or plants. These systems achieve large internal surfaces while allowing an optimized mass transport. This is used in plants to perform capillarity- induced motions, transport substances to reaction sites and remove educts from chemical processes. We are aiming to mimic such systems with artificially produced hierarchically porous silicon. The bimodal, hierarchical structure leads to a different imbibition behavior than porous systems with a monomodal pore-size distribution. Therefore, we used 2D finite element fluid dynamic simulations to achieve deeper insights into single-pore events and competing Laplace pressures in pore sections with distinct pore sizes. The simulations are related to the experimental results from dilatometry, mass-uptake and synchrotron-based, in-situ X-ray radiography imbibition experiments. This allows a complete description of the transport phenomena and will help us to tailor the material for applications in capillarity-driven pumps or energy harvesting from natural processes.

CPP 35.4 Thu 10:30 H 0107

Percolation in Networks of Liquid Diodes — Camilla Sammartino, Yair Shokef, and •Bat-El Pinchasik — Tel Aviv University, School of Mechanical Engineering, Israel

Liquid diodes are surface structures that facilitate the spontaneous flow of liquids in a specific direction. In nature, they are used to increase water collection and uptake, reproduction, and feeding. However, pump-free large networks with directional properties are exceptional and are typically limited up to a few centimeters. Here, we simulate, design, and 3D print networks consisting of hundreds of liquid diodes. We provide structural and wettability guidelines for directional transport of liquids through these networks and introduce percolation theory in order to identify the threshold between a connected network, which allows fluid to reach specific points, and a disconnected network. By constructing well-defined networks with uni- and bidirectional pathways, we experimentally demonstrate the applicability of models describing isotropically directed percolation. We accurately predict the network permeability and the liquid final state. These guidelines are highly promising for the development of structures for spontaneous, yet predictable, directional liquid transport. In addition, they comprise an initial realization of complex liquid circuits, analogoues to electric circuits.

CPP 35.5 Thu 10:45 H 0107

Wetting underneath droplets on an oily surface — •Shiva Moradimehr and Kirsten Harth — Fachbereich Technik, TH Brandenburg, Brandenburg a. d. Havel

When a liquid drop impacts on a smooth surface, a thin layer of air evolves between the drop and the surface. The drop deforms under the influence of the ambient air that needs to be squeezed out before the drop can touch the substrate. The actual air layer profile depends on the impact velocity, ambient gas, drop liquid as well as the deformability of the substrate. For small impact Weber number, the air film ruptures before drop rebound. The wetting front connecting the drop and layer liquids propagates at velocities of few meters per second.

We study the wetting front velocity for droplets impacting on hard substrates covered by thin oil layers using high-speed interferometry at oblique incidence. The impact velocity, viz. the thickness of the entrained air layer, and the oil layer properties are varied. Both a model for contact spreading on a thin film or an film-rupture based model are initial candidates to describe the wetting front propagation.

CPP 36: Organic Electronics and Photovoltaics III

Time: Thursday 9:30–13:00 Location: H 0110

CPP 36.1 Thu 9:30 H 0110

How 'Hot' are the Charges in OPV? — •Priya Viji, Constantin Tormann, Clemens Göhler, Dorothea Scheunemann, and Martijn Kemerink — IMSEAM, Universität Heidelberg, Germany

The question of whether charge transport in operational organic solar cells (OSC) occurs far-from-equilibrium or not is of practical and fundamental importance. While the equilibrium picture of the OSC assumes that the photogenerated charge carriers quickly lose their energy and attain lattice temperature, kinetic Monte Carlo (kMC) simulations of OSC have consistently shown that photogenerated charges are extracted before reaching thermal equilibrium energy: the population relaxes, albeit to an effective temperature that exceeds that of the lattice. In this work, we use Johnson thermometry to measure the temperature of the photogenerated carriers by noise spectroscopy. Two systems, P3HT:PCBM and PM6:Y6, are tested against their inorganic counterpart, silicon. The experiments prove, in contrast to silicon PV, charges in operational OSC are not thermalized and are almost twice as hot as the lattice. The experimental findings are confirmed by kMC simulations, which show that the energetic disorder in organic semiconductors is the reason for slow thermalization as well as high effective temperature. Our results imply that OSCs are far from equilibrium systems, which opens realistic prospects to mitigate the thermalization losses and eventually beat the near-equilibrium thermodynamic limit. In fact, the results show that a regular OSC is Hot-Carrier Solar Cell in the sense that excess energy contributes to output power.

CPP 36.2 Thu 9:45 H 0110

Energetic landscape of fluorinated and non-fluorinated donors and non-fullerene acceptors in bulk heterojunction organic photovoltaics — Shahidul Alam[1], Jafar I. Khan[2], Vojtech Nádaždy[3], Tomáš Váry[3], Aurelien D. Sokeng[4], Md Moidul Islam[4], Christian Friebe[4], Wejdan Althobaiti[1], Wenlan Liu[5], Martin Hager[4], Ulrich S. Schubert[4], Carsten Deibel[6], Denis Andrienko[5], Frédéric Laquai[1], and •Harald Hoppe[4] — [1]KAUST, Saudi Arabia — [2]University of Hull, UK — [3]Slovak Academy of Sciences, Slovak Republic — [4]IOMC/CEEC, Jena, Germany — [5]MPIP, Mainz, Germany — [6]TU Chemnitz, Germany

Performance improvement of OSCs via fluorination of the D and/or NFA is an effective method. The end-group fluorination of the well-known NFA ITIC yields further extension of the absorption to the NIR, which increases the SC's Jph compared to the non-fluorinated version. Herein, ITIC and two of its fluorinated variants were synthesized and systematically investigated concerning the influence of end-group fluorination on physicochemical, optical, and photovoltaic properties. DFT calculations show that fluorination increases the EA of the acceptor and, therefore, reduces the Voc of the built devices. On the other hand, the molecular quadrupole moment increases with the degree of fluorination leads to more efficient dissociation and reduced recombination of CT-states at the D-A interface. At the same time, IE increases, thus increasing the driving force for CT-state formation. The collected and presented results herein shed light on the importance of the energetic landscape at the D-A interface and how this deviates from general expectations when consulting the pristine materials.

CPP 36.3 Thu 10:00 H 0110

Optimizing Thermal Annealing Sequences for Enhanced Photovoltaic Performance in Organic Solar Cells — •Haya Aldosari[1,2], Shahidul Alam[1], José Jurado[1], and Frédéric Laquai[1] — [1]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 — [2]Department of Physics, College of Science, Imam Abdulrahman Bin Faisal University, P.O. Box 383, 31113, Dammam, Saudi Arabia

Thermal annealing is a widely used approach in organic solar cell research aimed at enhancing the performance of these devices. Therefore, the bulk heterojunction of PBDB-T:IT-2F was subjected to thermal annealing at various phases of the fabrication process to examine the impact of annealing on the photovoltaic characteristics. Several optoelectronic methods were employed to investigate the kinetics of charge recombination and the process of charge extraction. Based on the results of our investigation, it has been observed that both post-annealing and 2-stage-annealing methods contribute to the enhancement of fill factor and power conversion efficiency. However, the latter method has even greater advantages. Further research explores the impact of annealing on the hole transport layer (MoOx). The work function of MoOx was enhanced during the annealing process, leading to an increase in the internal electric field and a higher rate of charge carrier extraction. Finally, field-dependent charge generation processes were investigated using time-delayed collection field measurements.

CPP 36.4 Thu 10:15 H 0110

Role of energetic offset in low-offset organic solar cells and its effect on loss pathways — •Bowen Sun and Safa Shoaee — Institute of Physics and Astronomy, University of Potsdam, Germany

While efficient charge generation despite ultra-low energy offsets (down to 0 eV offsets) between donor and acceptor in non-fullerene acceptor (NFA) based organic solar cells (OSCs) has been often reported, the physical meaning of this observation is discussable and unclear.

In this work, we have performed advanced optoelectronic and morphology characterization, as well as optical simulation for a series of donor:NFA systems. The energetic offsets between CT and excitons, as well as the effect of this energetic offset on the carrier loss pathways in different bias conditions have been studied in detail. From our work, we reached several important conslusions: 1) the short circuit current density and fill-factor of low-offset systems are largely determined by a field-dependent exciton dissociation yield. 2) The energetic offset also affects the recombination dynamics. Our analysis clearly shows that this enhanced recombination is contributed by a highly non-radiative channel, indicating the significance of triplet states in the recombination process. 3) It is strongly indicated that the charge generation and recombination (losses) proceed via different energetic states. The losses during charge generation process occur via highly radiative channels, while that during charge recombination process proceed via highly non-radiative channels. In general, our study clarifies the role and effect of energetic offset in low-offset OSCs, and provides a guideline for the further improvement of OSCs.

CPP 36.5 Thu 10:30 H 0110

Photophysics of Poly(3-hexylthiophene): Non-Fullerene Acceptor Based Organic Solar Cells — •Wejdan Althobaiti, Julien Gorenflot, Catherine De Castro, Jafar Khan, Shahidul Alam, Christopher Petoukhoff, 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, Saudi Arabia

The efficiency of P3HT:Non-fullerene acceptor (NFA) based solar cells lacks considerably behind many other polymer donor:NFA systems. For reasons which are yet incomprehensible. Here, we report on a series of P3HT:NFA solar cells, and elucidate the origin of performance losses in terms of the photophysical processes. It is a matter of fact that the interfacial ionization energy (IE) offset is a critical parameter in NFA-based blends in determining the efficiency of the exciton-to-charge transfer (CT) state conversion. We show that while large IE offsets in excess of >0.9 eV still facilitate complete exciton quenching, the device internal quantum efficiency (IQE) is limited by geminate and / or non-geminate recombination processes in P3HT-based photoactive blends. Our finding shows a drop in IQE when the diagonal bandgap of the photoactive blend i.e the difference between the IE of the donor and the electron affinity (EA) of the acceptor is small irrespective of the IE offset. Understanding the relation between the IE offsets, EA offsets at the interface of donor and acceptor materials, and the performance of organic solar cells could improve the charge generation efficiency.

CPP 36.6 Thu 10:45 H 0110

Correlating the morphology of PTQ-2F:BTP-4F organic solar cells through scattering and real space methods — •Lukas V. Spanier[1], Julian E. Heger[1], Renjun Guo[1], Matthias Schwartzkopf[2], Harishankar Balakrishnan[3], Rachid Houssaini[3], Stephan V. Roth[2], Achim Hartschuh[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]LMU, Department Chemie und CeNS, 81377

Munich, Germany — [4]TUM, MLZ, 85748 Garching, Germany

Lately, organic solar cells (OSCs) have gained increasing attention due to their rapidly increasing efficiencies as well as the relatively easy scalability in their manufacture. To make the manufacturing process of the bulk-heterojunction (BHJ) more environmentally friendly, increased efforts have recently been made to use halogen-free solvents, which, however, can lead to reduced efficiencies.

We investigate the changes in morphology and performance stability of PTQ-2F:BTP-4F organic solar cells processed from various halogenated and non-halogenated solvents, utilizing operando grazing-incidence wide and small angle X-ray scattering (GIWAXS/GISAXS) during illumination and solar cell operation. We further show the impact of solvents on the mesoscopic distribution of small molecules within the bulk heterojunction through scattering-type scanning near-field optical microscopy.

CPP 36.7 Thu 11:00 H 0110

Polymer Donors vs. Small Molecule Donors for Solar Cells — •Elifnaz Sağlamkaya and Safa Shoaee — Disordered Semiconductor Optoelectronics, Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm, Germany

All small molecule (ASMs) solar cells have great potential to actualize the commercialization of organic photovoltaics owing to their higher solubility, lesser batch-to batch variety and simpler synthesis routes compared to the blend systems that utilize conjugated polymers. However, the efficiency of the ASMs are slightly lacking behind the polymer: small molecule single heterojunctions. To address this discrepancy, we compare a small molecule donor ZR1 and polymer PM7 blended with Y6 acceptor. Our temperature dependent electroluminescence quantum efficiency analysis reveals the same energetic offset between the charge transfer state and the singlet energy (ΔE_{S1-CT}) in PM7:Y6 and ZR1:Y6. Surprisingly, the ZR1:Y6 has noticeably stronger field-dependency of charge generation. Furthermore, the energy barrier for charge generation is quite high (100 meV) for the ZR1:Y6 system unlike the PM7:Y6 (10 meV). Low charge carrier mobilities of ZR1:Y6 measured from the space charge limited currents entail a viable explanation for energy barrier for the charge generation. On the other hand, the maximum power point tracking measurements show a higher stability of ZR1:Y6, exhibiting a tradeoff between efficiency and stability.

15 min. break

Invited Talk CPP 36.8 Thu 11:30 H 0110

Digital luminescence: Novel platform for minimalistic photonic applications based on programmable luminescent tags — •Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden, Dresden, Germany

Information is everywhere and with the ever-growing thirst for data in the digital age, solutions for information storage and exchange need to advance. Barcodes and QR-codes are the current systems for passive information distribution in all sectors (B2B, B2C, and private). In this talk, I will present an advanced system for information storage and exchange based on luminescence of organic molecules. In contrast to passive printed codes, these programmable luminescent tags (PLTs) allow for non-contact writing, erasing, and re-writing, thus allowing much more use scenarios where the interaction with the data is essential. The system's core functionality is based on the phosphorescence of organic emitters, which can be turned on or off depending on the presence or absence of nearby molecular oxygen, respectively. These emitters are embedded in special transparent polymer foils, rendering the PLTs invisible when not used. Following the discussion of the general concept of PLTs, I will give an update on our recent efforts towards such systems made from biodegradable materials to demonstrate their potential as environmentally-harmless functional systems.

CPP 36.9 Thu 12:00 H 0110

The Photocurrent in Organic Solar Cells does not Vanish at Open-Circuit — •Clemens Göhler, Mónica Dyreby, Alexander Flamm, and Martijn Kemerink — Institute for Molecular Systems Engineering and Advanced Materials, Universität Heidelberg, Im Neunheimer Feld 225, 69120 Heidelberg

Organic solar cells (OSCs) have reached close to 20% of power conversion efficiency and 100% conversion yield between incident photons to extracted charge carriers, but still suffer from unexpected losses to the open-circuit voltage and fill factor. Non-thermalized charge carrier distributions—due to incomplete relaxation in a disordered density of states—can explain their current-voltage-characteristics, yet with at times uncommon ramifications: here, we will show that a non-negligible photogenerated current under open-circuit conditions is a general feature of OSCs. In more detail, we have investigated the internal quantum efficiency in non-fullerene acceptor OSCs in the steady state. Utilizing a small signal light source, modulated at low frequencies, and varying the working conditions from reverse (collection) to forward (injection regime) fields, we are able to determine the extraction efficiency of photogenerated charges at any point on the current-voltage-curve. We find that while the yield decreases towards open-circuit, it does not vanish completely; therefore, the resulting photocurrent has to be compensated by charge injection in order to reach zero net current. We were further able to reproduce these experimental findings with kinetic Monte-Carlo device simulations involving non-equilibrium dynamics.

CPP 36.10 Thu 12:15 H 0110

Structure-function properties in a water soluble polymer via single-molecule spectroscopy — •Erik F. Woering[1], Maria Duma[1], Jane Kardula[1,2], Ryan C. Chieci[1,2], and Richard Hildner[1] — [1]University of Groningen, ZIAM, The Netherlands — [2]University of Groningen, Stratingh Institute for Chemistry, The Netherlands

Conjugated polymers represent a promising class of versatile and easy to produce high-performance materials. Due to their (chemically) adjustable nature, they find use in bioelectronics or organic solar cells. However, the interplay of the polymers' chemical structure of the backbone and of the side groups on optical and electronic properties remain largely unexplored due to their large conformational flexibility. Here, we perform temperature-dependent single-molecule photoluminescence (PL) spectroscopy on p(ProDOT-TetEster), a water-soluble polythiophene-derivative bearing two dimethyloctane-dioate side chains. In particular, we explore the influence of polarity of the surrounding environment through statistical analysis of spectral features upon embedding single chains into a PS, PMMA or PVA matrix. The granular analysis on the single-chain scale will be valuable for deriving structure-function relationships and ultimately for the design of optimized and specialized conjugated polymers.

CPP 36.11 Thu 12:30 H 0110

On the competition between exciton emission and free charge generation in organic solar cells with low energetic offsets — •Manasi Pranav[1], Atul Shukla[1], Bowen Sun[1], Rong Wang[2], David Moser[3], Julia Rumeney[3], Sander Smeets[4], Wouter Maes[4], Sabine Ludwigs[3], Larry Lüer[2], Christoph Brabec[2], Safa Shoaee[1], and Dieter Neher[1] — [1]University of Potsdam, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [3]University of Stuttgart, Germany — [4]Hasselt University, Belgium

Organic blends with low energy-offset are the fruit-flies of today's organic photovoltaics research. Low photocurrent efficiencies for low offset blends draw attention to the link between energetic offset and free charge generation. Here, we take a quantitative, methodical approach to probing the origin of field-dependent free charge generation. Blending Y6 and Y5 with different molecular weights of the PM6, we progressively tune the photovoltaic parameters from a very efficient to inefficient device with severe field dependence of generation. We find the same pronounced field-dependence in transient absorption spectroscopy, and steady state and transient photoluminescence (PL) for inefficient low offset blends. The free charge generation and PL show a strict anticorrelation as a function of bias across all model systems. Thereby, we theoretically evaluate the quantum yields of PL to demonstrate inefficient charge transfer state formation from the local exciton, without any indication of hybridization, and that the decay of the singlet exciton is the only competing process to free charge generation.

CPP 36.12 Thu 12:45 H 0110

Directed exciton transport highways in organic semiconductors — Kai Müller[1,2], Sebastian Schellhammer[1,3], Nico Grässler[3,4], Bipasha Debnath[4], Fupin Liu[4], Yulia Krupskaya[4], Karl Leo[3], Martin Knupfer[4], and •Frank Ortmann[1,5] — [1]cfaed, TU Dresden — [2]Institut für Theoretische Physik, TU Dresden — [3]IAPP and IAP, TU Dresden — [4]Leibniz Institute for Solid State and Materials Research Dresden — [5]TUM School of Natural Sciences, Technische Universität München

Exciton bandwidths and exciton transport are difficult to control by material design. We showcase the intriguing excitonic properties in an organic semiconductor material with specifically tailored functional groups, in which extremely broad exciton bands in the near-infrared-visible part of the electromagnetic spectrum are observed by electron energy loss spectroscopy and theoretically explained by a close contact between tightly packing molecules and by their strong interactions. This is induced by the donor-acceptor type molecular structure and its resulting crystal packing, which induces a remarkable anisotropy that should lead to a strongly directed transport of excitons. The observations and detailed understanding of the results yield blueprints for the design of molecular structures in which similar molecular features might be used to further explore the tunability of excitonic bands and pave a way for organic materials with strongly enhanced transport and built-in control of the propagation direction.

CPP 37: Biopolymers, Biomaterials and Bioinspired Functional Materials (joint session CPP/BP)

Time: Thursday 9:30–13:00 Location: H 0111

Invited Talk CPP 37.1 Thu 9:30 H 0111

Self-organized protein/polysaccharide nano-assemblies for applications in biomedical and food sciences — •Aristeidis Papagiannopoulos — Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vass. Constantinou Ave. 11635 Athens, Greece

Multifunctional nanocarriers of drugs and nutrients are very important for applications in the food industry and pharmaceutics. Proteins and polysaccharides are extensively used in these fields as they are biodegradable, metabolizable, nontoxic and biocompatible. Nanostructures from these two biopolymer classes combine the multifunctionality of the proteins (hydropathy and pH-dependent charge surface distributions) with the hydrophilicity and hydrogen-bonding property of the polysaccharides. Our recent work on protein/polysaccharide nanoparticles by electrostatic self-organization and thermal treatment without the use of chemical reactions or toxic solvents will be presented. Examples will include fibrinogen-hyaluronic acid nanoformulations, bovine serum albumin-chondroitin sulfate or -xanthan nanoparticles, trypsin- and hemoglobin-based nanoparticles. The discussion will be focused on the stimuli-response, molecular interactions and hierarchical morphology of the protein/polysaccharide systems and the binding of bioactive compounds. Physicochemical characterization and optimization of the nano-assemblies by light scattering, small angle scattering and spectroscopy techniques will be analyzed. These works motivate the development of other novel protein/polysaccharide biomaterials.

CPP 37.2 Thu 10:00 H 0111

Dichroic ATR-FTIR studies on thin bioinspired films of spider silk related peptide blends — Mirjam Hofmaier[1], •Thomas Scheibel[2], Andreas Fery[1], and Martin Müller[1] — [1]Leibniz Institute of Polymer Research Dresden (IPF), Institute of Physical Chemistry and Polymer Physics, 01069 Dresden, Germany — [2]University of Bayreuth, Chair of Biomaterials, 95447 Bayreuth, Germany

Bioinspired binary blends of a crystalline (C) and amorphous (A) peptide sequence were prepared addressing analogy to C-A multiblockcopolymer-like spider silk proteins. C/A blends were prepared in hexafluoroisopropanol for molar mixing ratios C/(C+A)=0, 25, 50, 77, 100%, deposited as thin films (d=31-44nm) onto silicon substrates and checked for secondary structure and orientation by dichroic transmission (T-) and ATR-FTIR spectroscopy. Amide I band analysis revealed little β-sheet (<15%) and much disordered (>79%) structure and dichroic ratios (R) of Amide I components indicating no β-sheet orientation for all C/(C+A) values. Whereas, after swelling in methanol vapor C/A blend films revealed increasing β-sheet up to 54% and decreasing disordered structure down to 42% with increasing C/(C+A). Furthermore, R values of Amide I components assigned to antiparallel beta-sheet were found by T-FTIR indicating no in-plane orientation, while ATR-FTIR revealed R values indicating significant out-of-plane orientation of β-sheet crystallites for blend films with C/(A+C)>0. SFM microscopy showed larger needle-like fibrillar structures for C/A blend films, while C-A copolymer films revealed smaller fibrillar or spherical structures correlating with the lower orientation obtained by ATR-FTIR.

CPP 37.3 Thu 10:15 H 0111

Exploring deposition conditions for antibacterial thin films via GISAXS measurements — •Joanne Neumann[1,2], Maria J Garcia[1,3], Holger Sondermann[1,3], Matthias Schwartzkopf[1], and Michael Martins[2] — [1]DESY, Photon Science, Notkestr. 85, D-22607 Hamburg — [2]UHH, Physics Department, Luruper Chaussee 149, D-22607 Hamburg — [3]CSSB, Center for Structural Systems Biology, Notkestr. 85, D-22607 Hamburg

During the last decades, the rate of multiresistant microbes against antibiotics increased dramatically. Moreover, biofilm-based contaminations complicate cleaning procedures and require cost-intensive methods in industrial processes. In this context, Pseudomonas aeruginosa (PA) is one of those bacteria that forms biofilms at liquid/air interfaces as a protective shell, e.g. against antibiotics. To investigate the influence of nanostructured silver layers as antibacterial coatings on the initial bacterial growth, we employed micro-focused Grazing incidence Small Angle X-ray Scattering (GISAXS) as a very surface-sensitive X-ray-based method providing structural information about electron density distributions. In our experiments we characterized PA biofilms, grown under different deposition conditions at the P03 beamline at Petra III / DESY.

CPP 37.4 Thu 10:30 H 0111

Colored CNC films reflect left and right circular polarized light. — •Silvia Vignolini — MPI Colloids and Interfaces Potsdam DE

The chiral self-assembly of nanoscale building blocks is a universal phenomenon that demonstrates the emergence of large-scale structures from the properties of individual sub-units. In many self-organising colloidal systems, such as cellulose nanocrystals (CNC), the emergence of chirality in the mesophase can be correlated to the properties of the building blocks and is therefore necessarily fixed. CNC chiral nematic suspensions are, in fact, always left-handed, giving rise when dried, to colored films reflecting only circular left-polarized light. In this talk, I will review some tricks that can be used to achieve CNC-colored films with circular right-polarized light reflection.

CPP 37.5 Thu 10:45 H 0111

Tailoring morphologies of protein-templated titania nanostructures — •Linus F. Huber[1], Stephan V. Roth[2], Manuel E. Scheel[1], and Peter Müller-Buschbaum[1,3] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Hamburg, Germany — [3]TUM, MLZ, 85748 Garching, Germany

Biotemplating is an effective technique for structuring hybrid inorganic-organic materials at the nano scale. This method facilitates the fine-tuning of material characteristics such as porosity and structure sizes. Therefore, parameters like the electronic conductivity can be adjusted for different applications. This work focuses on titania thin films with different structures, for their application in thermoelectric generators. Beta-lactoglobulin, a bovine whey protein, serves as a template in the sol-gel synthesis process. The Seebeck effect allows the conversion of waste heat into electrical energy. This research aims to address the scarcity, toxicity, and costliness of current state-of-the-art thermoelectric materials. To investigate the morphologies of titania, a combination of in situ GISAXS, GIWAXS, and SEM techniques are used. In particular, in situ GISAXS printing allows for a time-resolved exploration of the structure formation, domain sizes, and domain distances.These observed structural differences are subsequently correlated with measurements of the Seebeck coefficient, electrical conductivity and optical properties.

CPP 37.6 Thu 11:00 H 0111

Sustainable photonic glass pigments from brush block copolymers — •Zhen Wang[1], Ruiting Li[2], Richard Parker[1], and Silvia Vignolini[1,2] — [1]Yusuf Hamied Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, UK — [2]Department of Sustainable and Bio-inspired Materials, Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14476 Potsdam, Germany

Growing societal concerns over microplastic pollution and resource sustainability is driving the pigment industry to search for sustainable alternatives. One promising avenue is block copolymer (BCP), which is known to self-assemble into structurally coloured materials. However, its real-world application has been hindered by limited exploration into the suitability of biocompatible and (bio)degradable monomers. In this talk we will show that biocompatible BCPs can be self-assembled within emulsified microdroplets, which upon drying form microparticles with a porous photonic glass architecture. The colour from these pigments can be tuned by either the BCP properties or the fabrication conditions. Finally, the relationship between the microparticle morphology and its optical response was investigated for BCPs with similar composition but different thermal behaviour. This revealed the formation mechanism for the porous structure and allowed for a strategy to enhance colour purity.

15 min. break

CPP 37.7 Thu 11:30 H 0111

Reservoir computing with organic fiber networks — •Richard Kantelberg, Anton Weissbach, Peter Steiner, Peter Birkholz, Hans Kleemann, and Karl Leo — Technische Universität Dresden, Dresden, Germany

Reservoir computing (RC) is a promising paradigm for machine learning that utilizes dynamic systems, known as reservoirs, to process and analyze complex temporal data. Organic mixed ionic electronic conductors (OMIECs) have emerged as a novel class of materials with intriguing properties, such as their ability to exhibit both electronic and ionic conductivity, as well as their biocompatibility, flexibility, and low power consumption. These features make OMIECs particularly suitable for the development of unconventional computing architectures. Conducting fiber networks grown by field-directed polymerization have been proven to be a suitable candidate for, e.g., heartbeat or image classification tasks. However, the dependency between classification accuracy and device parameters is still rather unclear. We present recent findings interlinking electronic conductivity, system nonlinearity and reservoir size with the neuromorphic functionality and RC performance. The recent progress in reservoir computing using organic mixed ionic electronic provides valuable knowledge for the targeted development of fiber reservoirs. Given these findings, we are confident to further increase the classification accuracy by adopting the system to specific application scenarios, paving the way to future commercialization.

CPP 37.8 Thu 11:45 H 0111

Paper Fibers Beyond Saturation: μ-CT Analysis of Prolonged Structural Changes — •Maximilian Fuchs[1,2], Raimund Teubler[1,3], Daniel Kollreider[1,2], Maximilian Grillitsch[1,2], Ekaterina Baikova[1,2], and Karin Zojer[1,2] — [1]Institute for Solid State Physics, Graz University of Technology, Austria — [2]Christian Doppler Laboratory for Mass Transport through Paper — [3]Institute of Analytical Chemistry and Food Chemistry, Graz University of Technology, Austria

The uptake of water or dimethylsulfoxid (DMSO) by a cellulose-lignin based fiber network, in this case paper, is a complex interplay between capillary transport and sorption of these polar volatiles into the fibers. Microcomputed tomography (μ-CT) allows us to correlate this uptake with changes in the microstructure, with water and DMSO being offered either as a liquid or additionally via the gas phase to prevent capillary uptake. A pore network analysis of the 3D images shows that uptake from liquid and gas cause similar initial structural changes, although the fiber space and pore space between the fibers swells to different extents. Interestingly, fibers and pores continue to expand long after mass uptake from gas phase has ceased. This long-lasting expansion is most likely caused by an increasing amount of detached fibril bundles in the fiber wall.

CPP 37.9 Thu 12:00 H 0111

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, Darmstadt 64289, Germany

In human physiology, endothelial cells (ECs) form a lining inside blood vessels, which is essential for cell maturation and the development of capillary vessels. However, replicating this process ex vivo, especially ensuring the adequate adherence of ECs to the surfaces of 3D-printed artificial networks, presents a significant challenge. In this study, we focus on designing an effective mediator between the inner wall of the artificial network and endothelial cells that would remain mechanically stable against the flow of the nutrient solutions for cell maturation. Our strategy involves the use of Poly(N-isopropylacrylamide) (PNIPAM) microgels (MGs) as mediators for cell culturing surfaces. To enhance their attachment, we synthesized charged MGs and tested their adhesion on plasma-treated silicon (Si), glass, and 3D-printed polymeric surfaces. The MG particles were characterized based on their Zeta potential and hydrodynamic radius. To achieve rapid deposition, we employed spin coating to form a thin polymeric layer of MG particles on the substrates. We conducted atomic force microscopy (AFM) analyses and observed stable adhesion of MG particles on flat surfaces, even after water washing and exposure to mechanical stress. Moreover, we observed that these MG coatings yield superior endothelial cell adhesion and spreading compared to non-coated substrates.

CPP 37.10 Thu 12:15 H 0111

A Computational Investigation into the Oxidation of Cytosine Epigenetic Modifications — •Vasilii Korotenko[1] and Hendrik Zipse[2] — [1]Forschungszentrum Jülich, IEK-9 — [2]LMU München, Fakultät für Chemie und Pharmazie

Studying the (aut)oxidation of 5-methylcytosine (5mC) is crucial for understanding the dynamic control of DNA methylation - a pivotal epigenetic modification linked to gene expression, cellular differentiation, and disease development. In this work, the oxidizing properties of oxygen-centered radicals and the reducing properties of epigenetically modified cytosines were studied. The O-H bond dissociation energies BDE(O-H) were calculated for various alcohols using selected theoretical methods. BDE(C-H) and pKa values have been calculated for various oxidation product of 5mC. Special attention was paid to the equilibrium of the hydration reaction of 5-formylcytosine (5fC), because the corresponding hydrate product can be very easily oxidized. All this together allowed us to propose and thermodynamically evaluate the mechanism of the 5mC (aut)oxidation reaction. The (aut)oxidation of 5mC is unlikely to occur through initiation by triplet dioxygen or through unimolecular decomposition of hydroperoxides. In the proposal mechanism, neural molecules react with free radicals, transferring hydrogen atoms to create products with higher BDE values. The thermodynamics of the presented mechanism agrees with the experimental kinetics. We assume that the protonation ($pH < 7$) of oxidizable nucleic acids inhibits the (aut)oxidation process by increasing the BDE(C-H) values.

CPP 37.11 Thu 12:30 H 0111

Arylazopyrazole Amphiphiles as New Candidates for Photo-Induced Drug Delivery — •Ipsita Pani, Michael Hardt, Dana Glikman, and Björn Braunschweig — Institute of Physical Chemistry, University of Münster, 48149 Münster, Germany

Photo-responsive materials have been extensively explored to meet the demands for high precision drug delivery. Azobenzene-based amphiphiles have been the focal point of research in photo-responsive drug delivery systems. However, most azo amphiphiles suffer from low thermal stabilities of the cis-isomer. Consequently, the drug carriers are subjected to prolonged and periodic UV irradiation of high intensity for the release of the encapsulated drug. Therefore, the design of nanocarriers for light-induced drug delivery demands innovations to achieve targeted release at low intensities and short exposure times of the UV irradiation. Arylazopyrazoles (AAPs) have emerged as novel photoswitches with superior thermal stability of the cis-isomer and photo-stationary states (>90%) for trans/cis photo-isomerization in both directions.[1,2] In this contribution, we report on the potential of an anionic AAP surfactant (octyl arylazopyrazole butyl sulfonate) as a micellar nanocarrier for doxorubicin which is the most widely used anti-cancer drug. Using surface specific tools such as surface tensiometry and vibrational sum-frequency generation (SFG) spectroscopy we demonstrate the UV-induced release of doxorubicin at the air-water interface, while the release of doxorubicin in aqueous solution is studied by UV-visible and fluorescence spectroscopy. [1] Hardt et al. *Langmuir* **2023**, 39, 5861 [2] Honnigfort et al. *Chem. Sci.* **2020**, 11, 2085

CPP 37.12 Thu 12:45 H 0111

Untangling the stabilizing effects of proteins as foaming

agents — •Kevin Gräff[1], Sebastian Stock[1], Luca Mirau[1], Sabine Bürger[1], Larissa Braun[1], Annika Völp[2], Norbert Willenbacher[2], and Regine von Klitzing[1] — [1]Soft Matter at Interfaces, Technische Universität Darmstadt, Darmstadt, Germany — [2]Institute of Mechanical Engineering, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Foams appear in many applications such as in personal care products, firefighting and food technology. Macroscopic foams consist of air bubbles separated by foam films. Therefore, it is crucial to untangle electrostatic, steric and network stabilization effects in foam films to understand macroscopic foam properties. We compare globular proteins (β - lactoglobulin and bovine serum albumin), a flexible protein (whole casein) and lupine protein isolate with varying solution pH. In a Thin Film Pressure Balance (TFPB) we use image intensity measurements to record spatially resolved disjoining pressure isotherms and to gain information about structure formation. We introduce feature tracking as a novel method to measure the interfacial mobility and stiffness of foam films. Around the isoelectric point, stable Newton Black Films (NBFs) for the globular proteins form in contrast to the unstable NBFs for the flexible proteins due to different characteristics of the network structures. To evaluate the foam films impact on macroscopic foams, we use a Bikerman cell to measure foam parameters (e.g. foamability). Small Angel Neutron Scattering (SANS) on macroscopic foams completes the picture.

CPP 38: Active Matter IV (joint session DY/BP/CPP)

Time: Thursday 9:30–13:00 Location: BH-N 334

Invited Talk CPP 38.1 Thu 9:30 BH-N 334
Flocking by turning away — •Ricard Alert — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Flocking, as paradigmatically exemplified by birds, is the coherent collective motion of active agents. As originally conceived, flocking emerges through alignment interactions between the agents. Here, I will show a new mechanism of flocking based on interactions that reorient agents away from each other. Combining simulations, kinetic theory, and experiments, we demonstrate this mechanism of flocking in self-propelled Janus colloids with stronger repulsion on the front than on the rear. We show that, unlike for alignment interactions, the emergence of polar order from turn-away interactions requires particle repulsion. The polar flocking state is stable because particles achieve a compromise between turning away from left and right neighbors. These findings could help to reconcile the observations that cells can flock despite turning away from each other via contact inhibition of locomotion. Overall, our work shows that flocking is a very robust behavior that arises even when the orientational interactions seem to prevent it.

CPP 38.2 Thu 10:00 BH-N 334
Metastability of ordered phase in discretized flocking — •Swarnajit Chatterjee[1], Mintu Karmakar[2], Matthieu Mangeat[1], Raja Paul[2], and Heiko Rieger[1] — [1]Center for Biophysics & Department for Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany. — [2]School of Mathematical & Computational Sciences, IACS, Kolkata – 700032, India.

Polar flocks are observed in a large class of active matter systems and have been considered robust to fluctuations. However, recent studies have argued that liquid polar flocks are metastable to the presence of small obstacles [1] or to the nucleation of opposite-phase droplets [2]. In this work, we study the stability of the ordered phase in flocking models with q-fold symmetry under the influence of counter- or transversely-propagating droplets. We observe that the liquid phase is more susceptible to a transversely-propagating droplet than a counter-propagating droplet. Also, for droplet counter-propagation, system morphology is dominated by a novel *"sandwich state"* of the liquid state and the droplet state rather than a reversal of the liquid phase. Here spatial anisotropy plays a crucial role. Metastability of the liquid phase in a discretized Vicsek model shows a strong dependency on the noise strength where the anisotropy parameter q does not significantly affect the reversal dynamics. Our study further investigates the influence of droplet size, density, and other control parameters on liquid stability.

[1] Codina et al., PRL 128, 218001 (2022).
[2] Benvegnen et al., arXiv:2306.01156 (2023).

CPP 38.3 Thu 10:15 BH-N 334
Emergent Metric-like States of Active Particles with Metric-free Polar Alignment — Yinong Zhao[1], Cristian L. Huepe[2], and •Pawel Romanczuk[3,4] — [1]Shanghai Jiao Tong University, Shanghai, PR China — [2]Northwestern University, Chicago, USA — [3]Department of Biology, Humboldt Universität zu Berlin, Germany — [4]Excellence cluster "Science of Intelligence", Berlin

We study a model of self-propelled particles interacting with their k-nearest neighbors through polar alignment. By exploring its phase space as a function of two nondimensional parameters (scaled alignment strength g and Peclet number Pe), we identify two distinct order-disorder transitions. One appears to be continuous, occurs at a low critical g value independent of Pe, and resembles a mean-field transition with no density-order coupling. The other is discontinuous, depends on a combined control parameter involving g and Pe, and results from the formation of small, dense, highly persistent clusters of particles that follow metric-like dynamics. These dense clusters form at a critical value of the combined control parameter Pe/g^{α} , with $\alpha \approx 1.5$, which appears to be valid for different alignment-based models. Our study shows that models of active particles with metric-free interactions can produce characteristic length-scales and self-organize into metric-like collective states that undergo metric-like transitions.

CPP 38.4 Thu 10:30 BH-N 334
Strong Casimir-like Forces in Flocking Active Matter — •Giuseppe Fava[1,2], Andrea Gambassi[3], and Francesco Ginelli[1,2] — [1]Dipartimento di Scienza e Alta Tecnologia and Center for Nonlinear and Complex Systems, Università degli Studi dell'Insubria, Como, Italy — [2]INFN sezione di Milano, Milano, Italy — [3]SISSA International School for Advanced Studies and INFN, via Bonomea 265, 34136 Trieste, Italy

Confining in space the equilibrium fluctuations of statistical systems with long-range correlations is known to result into effective forces on the boundaries.

In this work we demonstrate the occurrence of Casimir-like forces in the non-equilibrium context provided by flocking active matter. In particular, we consider a system of aligning self-propelled particles in two spatial dimensions, which are transversally confined by reflecting or partially reflecting walls. We show that in the ordered flocking phase this confined active vectorial fluid is characterized by extensive boundary layers, as opposed to the finite ones usually observed in confined scalar active matter. A finite-size, fluctuation-induced contribution to the pressure on the wall emerges, which decays slowly and algebraically upon increasing the distance between the walls.

We explain our findings which display a certain degree of universality within a hydrodynamic description of the density and velocity fields.

Ref: "Strong Casimir-like Forces in Flocking Active Matter", arXiv:2211.02644

CPP 38.5 Thu 10:45 BH-N 334
Collective Dynamics in Dense Systems of Active Polar Disks — •yating zheng[1,2], weizhen tang[3], amir shee[4], pawel romanczuk[1,2], and cristian huepe[4] — [1]Humboldt-Universität zu Berlin — [2]Research Cluster of Excellence 'Science of Intelligence' — [3]Beijing Normal University — [4]Northwestern University

We study a general model of a dense system of active polar disks with repulsive linear interactions, confined by a circular boundary. Each disk advances with a preferred self-propulsion speed and changes heading by turning around an axis of rotation located at a distance R behind its barycenter. We characterize the emerging phases and collective states as a function of R, density, and noise, for disks with isotropic and anisotropic damping disks, and a smooth or rough boundary. We find a rich phase space that combines transitions from solid to fluid states with novel R-dependent transitions from a collective state displaying localized disk rotation to a milling state around a common centre of rotation. These transitions are related to the formation of vortices that follow simple or complex dynamics depending on the boundary properties and system size. Our results demonstrate generic collective states that are expected to be observed in experimental dense systems of natural or artificial active agents in confined spaces.

CPP 38.6 Thu 11:00 BH-N 334

Cooperative resetting exhibits a delocalisation phase transition — •Felix J. Meigel and Steffen Rulands — Arnold Sommerfeld Center for Theoretical Physics, Department of Physics, Ludwig-Maximilians-Universität, München, Germany

In the realm of biology, many non-equilibrium systems are inherently noisy, while their proper functioning relies on the adept control of fluctuations. Stochastic resetting processes, where the state of a system is reset to its initial condition at random times, provide a framework for the control of the accumulation of fluctuations over time. Yet, in this framework, resetting is externally imposed. Here, we demonstrate that a constraint of fluctuations can also be achieved in a self-organized manner by cooperative resetting in many-particle systems. Specifically, we demonstrate that many-particle systems, wherein pairs of particles are reset to their respective average positions, exhibit a second-order phase transition as a function of the resetting rate. This transition delineates a regime where particles localize, thereby controlling fluctuations, and another regime where particle positions become unbounded. Our research showcases that cooperative resetting enables adaptation to external perturbations and enhances the optimization of search tasks compared to extrinsic resetting. We showcase the versatility of self-organized fluctuation control through cooperative resetting, with applications ranging from biological systems, such as intracellular vesicle dynamics and the fitness advantages of genetic recombination, to technical domains like the optimization of shared mobility services.

15 min. break

Invited Talk CPP 38.7 Thu 11:30 BH-N 334

Growth and division as drivers of complex dynamics in dense cellular matter — •Philip Bittihn — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

Cells in systems such as tissues, bacterial aggregates, embryonic development or tumors self-organize on large scales to fulfil their biological functions. Many such collective behaviors have been studied in the broader context of active matter, where they emerge from the intrinsic non-equilibrium activity of the constituent particles. Growth and division as drivers of activity have received less attention, although they are defining features of life and often play indispensable roles.

Here, I will describe some of our recent theoretical efforts in characterizing their effects in dense cellular matter. Using minimal models of mechanically interacting particles, we investigate scenarios in which growth and division either lead to large-scale flows and volume expansion or total volume is conserved. By developing statistical descriptions suited for non-conserved particle numbers, we find that certain components of particle motion follow simple scaling laws that can be related to macroscopic flows or to classical active particle models. Other features of the dynamics reveal new phenomena and transitions due to growth-induced pressure, confinement and anisotropic particle shapes. If time permits, I will outline interactions with motility or chemical activity. Overall, our results aim to establish universal physical principles as a baseline for experimental observations and provide design strategies for bio(technological) applications or artificial systems.

CPP 38.8 Thu 12:00 BH-N 334

Motility-induced clustering of active particles under soft confinement — •Timo Knippenberg[1], Ashreya Jayaram[2], Thomas Speck[2], and Clemens Bechinger[1] — [1]FB Physik, Universität Konstanz, Deutschand — [2]Institute for theoretical physics IV, Universität Stuttgart, Deutschland

In the field of active matter, motility-induced phase separation (MIPS) is one of the most widely studied subjects. This phenomenon, characterized by a phase transition from a homogeneous phase into a densely clustered state with a gaseous surrounding, occurs at sufficiently high density and active particle (AP) velocity. However, most of these studies focus on APs in bulk or near hard walls, while research on APs in soft confinement is scarce. The latter promises insights into the dimensionality-dependent aspects of MIPS, as gradually increasing the confinement strength provides a way to approach the 1-dimensional limit, where MIPS is known to be absent.

To address this topic, here we experimentally investigate the structural and dynamical properties of APs confined in a soft annulus-shaped channel. Depending on the strength of the confinement and the AP velocity, we observe a novel re-entrant phase behavior. We can explain our measurements by the strong coupling between velocity and the effective confining dimensionality in such soft systems.

In addition to highlighting the important influence of soft boundaries on APs, our research has implications for future applications in micro-robotics.

CPP 38.9 Thu 12:15 BH-N 334

Emergent memory from tapping collisions in active granular matter — •Lorenzo Caprini, Anton Ldov, René Wittmann, Christian Scholz, and Hartmut Löwen — Heinrich-Heine University of Düsseldorf

In an equilibrium thermal environment, random elastic collisions between the background particles and a tracer establish the picture of Brownian motion fulfilling the Einstein relation between diffusivity and mobility. In nature, environments often comprise collections of autonomously moving objects, termed active matter, which exhibit fascinating phenomena. We investigate experimentally the impact of an active environment on a passive tracer by using active granular particles, i.e. vibrationally excited inertial self-propelled units termed vibrobots. They display multiple correlated tapping collisions with the tracer, by bouncing and sliding on its surface. As a consequence, the tracer displays a persistent memory and is described by a generalized active Einstein relation that constrains fluctuations, dissipation, and effective activity due to the tracer memory. Since the resulting persistence can be tuned by the environmental density and motility, our findings can be useful for engineering properties of various active systems in biomedical applications and swarm robotics.

CPP 38.10 Thu 12:30 BH-N 334

Stationary particle currents in sedimenting active matter wetting a wall — •Matthieu Mangeat, Shauri Chakraborty, Adam Wysocki, and Heiko Rieger — Saarland University, Saarbrücken, Germany

Recently it was predicted, on the basis of a lattice gas model, that scalar active matter would rise against gravity up a confining wall in spite of repulsive particle-wall interactions [PRL 124, 048001 (2020)]. We confirm this prediction with sedimenting active Brownian particles (ABPs) in a box and elucidate the mechanism leading to the formation of a meniscus rising above the bulk of the sedimentation region. The height of the meniscus increases algebraically with the activity, and the formation of the meniscus is determined by a stationary circular particle current centered at the base of the meniscus. The origin of these vortices can be traced back to the confinement of the ABPs in a box: already the stationary state of non-interacting ABPs without gravitation displays highly symmetric circular currents. Gravitation distorts this vortex configuration downward, leaving two major vortices at the two side walls, with a strong downward flow along the walls. Repulsive interactions between the ABPs change this situation only as soon as motility induced phase separation (MIPS) sets in and forms a dense, sedimented liquid region at the bottom, which pushes the center of the vortex upwards towards the liquid-gas interface. Self-propelled particles therefore represent an impressive realization of scalar active matter that forms stationary particle currents being able to perform visible work against gravity, which we predict to be observable experimentally.

CPP 38.11 Thu 12:45 BH-N 334

Velocity-density scaling for active particles in an external field — •Colin-Marius Koch and Michael Wilczek — Theoretical Physics I, University of Bayreuth, Germany

Active particles in external fields can show diverse aggregation phenomena. The emerging collective phenomena and their statistics can thereby depend on microscopic details of active constituents' interactions. Here, we investigate how different steric interactions and self-propulsion mechanisms affect the aggregation of active particles in an external field. While density and velocity profiles individually differ between the studied cases, they consistently scale inversely with each other, when the instantaneous velocity projected onto the particle orientation is considered. The observed velocity-density scaling is robust for relatively dilute systems in which no strong aggregation, i.e. motility-induced phase separation, is present. We conclude that different microscopic details can result in the same statistics of collective behaviour in systems that are dilute enough.

CPP 39: Focus Session: Ultrafast Processes in Organic Semiconductors and Perovskites I (joint session O/CPP)

The fundamental processes determining the fate of excitons or charge carriers in organic semiconductors or perovskites are happening on an ultrafast timescale, i.e. 100 fs to 10 ps. This, for example, includes singlet-fission, excimer and polaron formation or hot carrier relaxation. Thus, for the development of efficient opto-electronic devices a deep understanding of the processes on this time scale is of utmost importance. Most importantly, theoretical and experimental methods must be combined to successfully decipher the studied phenomena as the many degrees of freedom in these soft matter materials often defy a straightforward explanation from the data. This Focus Session brings together theoretical and experimental scientists fostering an exchange of ideas on the various computational and experimental methods of the ultrafast sciences to the field of organic semiconductors and perovskites.

Organizers: Sebastian Hammer (U Montreal), Petra Tegeder (U Heidelberg)

Time: Thursday 10:30–13:00 Location: MA 004

Topical Talk CPP 39.1 Thu 10:30 MA 004

Transport and trapping in molecular materials at the picosecond time scale — •Marina Gerhard — Department of Physics and Material Sciences Center, Philipps-Universität Marburg, Germany

The Excitonic character of photoexcited states and the soft lattice of organic semiconductors pose guidelines for the design of devices, which are substantially different from those of their inorganic counterparts. To exploit the benefits of organic semiconductors, it is essential to comprehend the fate of photogenerated excitons at early times after their generation. In this context, molecular materials with a well-defined structure serve as ideal model systems to study processes such as exciton transport, excimer formation, singlet fission and energetic funneling. This contribution focuses on two recent studies, in which we explore the exciton dynamics in molecular systems using time and spatially resolved photoluminescence spectroscopy. For tetracene, the transport of excitons is driven by the interplay between singlet fission and triplet fusion. We demonstrate that this peculiar transport mechanism shows a pronounced temperature dependence and that it is severely hampered by the presence of trap states. The second study investigates heterostructures comprised of anthradithiophene with small concentrations of pentacene, which can efficiently mediate singlet fission through a favorable energy level arrangement of both compounds, demonstrating a system in which exciton funneling opens the possibility to spatially and spectrally separate light harvesting and singlet fission moieties.

CPP 39.2 Thu 11:00 MA 004

Fluctuations and exciton dynamics in molecular semiconductors — •Alexander Neef[1], Samuel Beaulieu[2], Sebastian Hammer[3], Shuo Dong[4], Tommaso Pincelli[1,5], Julian Maklar[1], R.Patrick Xian[6], Anke Krueger[7], Martin Wolf[1], Laurenz Rettig[1], Jens Pflaum[8] und Ralph Ernstorfer[1,5] — [1]Fritz-Haber-Institut — [2]Centre Lasers Intenses et Applications (CELIA) — [3]McGill University — [4]Chinese Academy of Sciences — [5]Technical University Berlin — [6]University of Toronto — [7]University of Stuttgart — [8]University of Wuerzburg

Time- and angle-resolved photoemission spectroscopy (trARPES) is a cutting-edge technique to study the electronic structure of materials out-of-equilibrium. Advances in instrumentation now allow taking multidimensional photoemission data sets of delocalized electrons in conventional semiconductors and the reconstruction of spatially confined molecular orbitals. I will present our recent results on trARPES studies of the fluctuation-dominated electronic structure of molecular semiconductors. Furthermore, I will talk about how trARPES made it possible to decipher a complex multiexcitonic process: singlet exciton fission [1]. Apart from the answers gained, a pressing question emerged: how can singlet exciton fission go uphill in energy in certain systems? Our work highlights the need for theories that are able to capture the behavior of excited states in a fluctuating landscape.

[1] Neef et al., Nature 616 (2023) https://www.nature.com/articles/s41586-023-05814-1

CPP 39.3 Thu 11:15 MA 004

Efficient Intramolecular Singlet Fission in Weakly-Interacting Heterodimers — •Oskar Kefer[1], Lukas Ahrens[2], Jie Han[3], Jan Freudenberg[2], Frank Rominger[2], Andreas Dreuw[3], Uwe H. F. Bunz[2], and Tiago Buckup[1] — [1]PCI, Universität Heidelberg, Heidelberg — [2]OCI, Universität Heidelberg, Heidelberg — [3]IWR, Universität Heidelberg, Heidelberg

Intramolecular singlet fission (iSF) converts one excited singlet (S_1S_0) into two triplets when two chromophores are covalently bound by a bridge. The bridge also determines the strength of intramolecular interaction. Usually, strong interaction leads to fast formation of the intermediate correlated triplet-pair ($^1[T_1T_1]$), but also hinders its dissociation. A Spiro-linker enforces a perpendicular π-system-arrangement around the central spiro-carbon, leading to long triplet-lifetimes that favor separation into T_1+T_1 without compromising $^1[T_1T_1]$-formation efficiency.

We expand on this approach and demonstrate a new class of heterodimers that exploit the favorable properties of spiro-conjugation with enhanced iSF dynamics. Quantum-chemical calculations (DFT) and transient absorption spectroscopy link accelerated iSF-kinetics to changes in the S_1S_0- and $^1[T_1T_1]$-energy landscape. The limited interaction during the lifetime of $^1[T_1T_1]$ creates favorable conditions for triplet-separation, which are formed with a yield of up to 174%. This new approach furnishes efficient heterogeneous iSF materials with reduced intramolecular interaction due to spatial fixation between chromophores and large, tunable absorption bandwidths.

Topical Talk CPP 39.4 Thu 11:30 MA 004

Ultrafast charge-transfer dynamics in organic and hybrid interfaces from first principles — •Caterina Cocchi — Institut für Physik und CeNaD, Carl von Ossietzky Universität Oldenburg

Charge-transfer dynamics at interfaces in the sub-ps timescale is ruled by complex interplays of electronic and vibrational degrees of freedom. First-principle methods based on real-time time-dependent density functional theory in conjunction with Ehrenfest dynamics offer a practical tool to access and rationalize these phenomena in realistic systems. Considering different organic and hybrid interfaces [1-3], I will discuss the mechanisms ruling charge-transfer dynamics triggered by a resonant pulse. I will illustrate how the intrinsic characteristics of the involved compounds and their mutual interactions affect qualitatively and quantitatively the dynamics of charge carriers in the earliest stages of light-driven coherent excitations. I will highlight methodological aspects that are necessary to reproduce the physics involved [4-6] and point out open issues to be addressed by future developments.

[1] M. Jacobs et al., Adv. Phys. X 5, 1749883 (2020). [2] M. Jacobs et al., ACS Appl. Nano Mater. 5, 5187 (2022). [3] M. Jacobs et al., J. Phys. Chem. A 127, 8794 (2023). [4] J. Krumland et al., J. Chem. Phys. 153, 054106 (2020). [5] J. Krumland et al., Phys. Rev. B 106, 144304 (2022). [6] M. Jacobs et al., arXiv:2311.01776

CPP 39.5 Thu 12:00 MA 004

Charge separation in a porphyrin-based metal organic framework incorporating C_{60} fullerenes — •Martin Richter[1], Xiaojing Liu[2], Pavel Kolesnichenko[1], Christof Wöll[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, Im Neuenheimer Feld 253/229, 69120 Heidelberg, Germany — [2]Institut für Funktionelle Grenzflächen, Karlsruher Institut für Technologie, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Porphyrin-based materials are attracting great interest due to their wide range of applications. They are often embedded into metal organic frameworks (MOF) to manipulate and investigate the relations between function and structure. Together with an electron acceptor charge separation can be achieved being beneficial for uses e.g. in solar cells or photocatalysis. Experiments on ZnTPP (Zinc 5,15-bis-(3,4,5-trimethoxyphenyl)-10,20-bis-(4-carboxyphenyl)) in a surface anchored MOF (SURMOF) loaded with fullerene C_{60} inside the pores have shown that photoexcitation increases the conductivity by up to two orders of magnitude.[1] Here, we investigate excited states dynamics after optical excitation with transient absorption spectroscopy on the femto- to nanosecond scale. Charge separated states can be identified, which have a lifetime of a few hundred picoseconds. The charge separation occurs after excitation of both the Soret band and the Q band.

1. X. Liu, Angew. Chem. Int. Ed. 2019, 58, 9590.

CPP 39.6 Thu 12:15 MA 004

Ultrafast charge separation and band structure dynamics in metal-phthalocyanine/WSe_2 heterostructures — •Gregor Zinke, Sebastian Hedwig, Benito Arnoldi, Martin Anstett, Martin Aeschlimann, and Benjamin Stadtmüller — University of Kaiserslautern-Landau, Germany

2D-Van-der-Waals materials and their heterostructures are a highly promising class of materials due to their low dimensional nature and diverse electronic properties, especially regarding their charge and spin carrier dynamics. In addition to chemical tunability, the spin-dependent electronic properties of such 2D heterostructures can also be altered on ultrafast timescales by the formation of transient charge-separated states. In this contribution, we focus on optically induced interlayer charge and spin transfer processes in heterostructures consisting of molecule films on the surface of a bulk WSe_2 crystal. Using spin-, time- and angle-resolved photoemission with XUV radiation, we can simultaneously monitor the excited carriers as well as the corresponding hole dynamics. For molecule films made of the metal phthalocyanines (MPcs) CuPc and FePc, we discuss the temporal evolution of optically excited spin and charge carriers in these MPc /WSe_2 heterostructures. We will illustrate the influence of the distinct orbital character of the central metal atom and structural order of the MPc molecules on the ultrafast electron and hole dynamics at the MPc/WSe_2 interface and discuss their impact on the transient changes in the interfacial energy level alignment.

CPP 39.7 Thu 12:30 MA 004

Disentangling the multiorbital contributions of excitons by photoemission exciton tomography — •G. S. Matthijs Jansen[1], Wiebke Bennecke[1], Andreas Windischbacher[2], Ralf Hemm[3], David Schmitt[1], Jan Philipp Bange[1], Christian Kern[2], Daniel Steil[1], Sabine Steil[1], Marcel Reutzel[1], Martin Aeschlimann[3], Peter Puschnig[2], Benjamin Stadtmüller[3,4], and Stefan Mathias[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Institute of Physics, University of Graz — [3]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern — [4]Institute of Physics, Johannes Gutenberg-University Mainz

The opto-electronic response of organic semiconductors is well-known to be dominated by excitons, i.e. quasiparticles that consist of bound electron-hole pairs. As excitons are realizations of a correlated many-particle wave function, experimental and theoretical methods must probe and characterize the the full electron-hole wavefunction, rather than just the single-particle orbitals. Recently, we have shown that time-resolved photoemission momentum microscopy can probe the entangled wavefunction and thereby unravel the exciton's multiorbital electron and hole contributions [1]. We demonstrate this for the prototypical organic semiconductor buckminsterfullerene (C_{60}) and achieve unprecedented access to key properties of the exciton state including localization, charge-transfer character, and ultrafast exciton formation and relaxation dynamics.

[1] W. Bennecke et al., arXiv preprint arXiv:2303.13904 (2023)

CPP 39.8 Thu 12:45 MA 004

Formation of charge-transfer excitons across the hybrid PTCDA/WSe_2 interface — •Wiebke Bennecke[1], David Schmitt[1], Jan Philipp Bange[1], Ignacio Gonzalez Oliva[2], Anna Seiler[1], Lukas Renn[1], Mattis Langendorf[1], Daniel Steil[1], Sabine Steil[1], R. Thomas Weitz[1], Peter Puschnig[3], Claudia Draxl[2], Marcel Reutzel[1], G. S. Matthijs Jansen[1], and Stefan Mathias[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Institut für Physik, Humboldt-Universität zu Berlin — [3]Institute of Physics, University of Graz

Heterostructures consisting of van-der-Waals materials and organic molecules are a promising material platform due to their potential to combine the flexibility of organic chemistry with the remarkable opto-electronic properties of 2D materials. Here, we use femtosecond photoemission momentum microscopy to study ultrafast exciton dynamics in monolayer PTCDA adsorbed on WSe_2. By employing the concepts of photoemission orbital tomography, which has recently been shown to be capable of capturing key excitonic properties [1, 2], we are able to unambiguously identify the different excitonic states formed after optical excitation of WSe_2. We find that a localized long-lived charge-transfer exciton is formed on a picosecond timescale, where the hole resides in the WSe_2 and the electron is being transferred to the lowest unoccupied molecular orbital of PTCDA.

[1] C. Kern et al., Phys. Rev. B **108**, 085132 (2023)

[2] W. Bennecke et al., arXiv preprint arXiv:2303.13904 (2023)

CPP 40: Focus Session: Novel Approaches to Surface Plasmon Generated Charges and Heat for Photocatalysis II (joint session O/CPP)

Time: Thursday 10:30–13:15 Location: MA 141

Topical Talk CPP 40.1 Thu 10:30 MA 141

Designing Plasmonic Photocatalysts — •Emiliano Cortes — Nanoinstitute Munich, Faculty of Physics, University of Munich (LMU), Munich, Germany

Nanostructured surfaces and colloids with designed optical functionalities - such as plasmonic & photonic nano and metamaterials - allow efficient harvesting of light at the nanoscale. Exploiting light-driven matter excitations in these artificial materials opens up a new dimension in the conversion and management of energy at the nanoscale [1-4]. One example are plasmonic and photonic catalysts, that can indeed confine solar energy into molecular regions [4-11]. In this talk, I will present our recent efforts in order to understand the light-matter interaction in plasmonic nanoparticles and metamaterials for photocatalysis [1-11].

References [1] E. Cortés, Nature 614, 230-232 (2023) [2] E. Cortés, et al. Nature Rev. Chem., 6, 259-274 (2022) [3] E. Cortés, et al. Chem. Rev. 122, 15082-76 (2022) [4] S. Ezendam, et al. ACS Energy Letters, 7, 778-815 (2022) [5] M. Herran, et al. Adv. Funct. Mat., 2203418 (2022) [6] J. Gargiulo, et al. Nature Communications 14, 3813 (2023) [7] L. Nan, et al. Nano Letters 23 (7), 2883-2889 (2023) [8] A. Stefancu, et al. ACS Nano 17 (3), 3119-3127 (2023) [9] L. Hüttenhofer, et al., Adv. Energy Mat., 46, 2102877 (2021) [10] M. Herran, et al. Nature Catalysis, accepted (2023) [11] S. Ezendam, et al. ACS Nano, accepted (2023)

CPP 40.2 Thu 11:00 MA 141

Plasmon assisted Catalytic Conversion of CO2 with Disordered Cu-Pd Network — •Oliver Wipf[1], Jelena Wohlwend[1], David Kiwic[2], Markus Niederberger[2], Ralph Spolenak[1], and Henning Galinski[1] — [1]Laboratory for Nanometallurgy, ETH Zürich, Switzerland — [2]Laboratory for Multifunctional Materials, ETH Zürich, Switzerland

The catalytic conversion of carbon dioxide is currently at the forefront of research as a way to mitigate the climate crisis by capturing CO2 and turning it into functional chemical components. However, currently this is a high energy consumption process, thus, developing efficient catalysts is critical. Using solar radiation to drive and catalyze chemical reactions could address this challenge. Here, we explore the plasmon assisted catalytic conversion of CO2 with disordered network metamaterials (DNMs). DNMs are an emerging class of metamaterials with tunable quasi-perfect absorption over a broad range of wavelengths. The optical response of such disordered networks can be conceptualized as coupled dipole-like networks, where the disorder of the metallic network traps and localizes surface plasmon (SP) waves.

In this work we harness DNMs as a platform to drive the conversion of CO2 by taking advantage of "hot" carriers, i.e. electron-hole (e-h) pairs, resulting from the non-radiative decay of plasmons. The generation of hot carriers is dependent on the chemistry and the local geometry, both tailorable with our fabrication route. Furthermore, we show that through chemical engineering of the DNMs, selectivity of the reaction products can be achieved.

CPP 40.3 Thu 11:15 MA 141

Advancing Plasmonic Charge Transfer for Photocatalysis: Bottom-Up Strategies in Energy Harvesting and Optoelectronics — •Swagato Sarkar[1] and Tobias A. F. Koenig[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Straße 6, 01069 Dresden — [2]Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, Helmholtzstraße 18, 01069 Dresden

Our study comprehensively explores bottom-up techniques for plasmonic charge transfer, focusing on their collective applications in energy harvesting. Extending the concepts of plasmon-photon hybridization to self-assembled plasmonic nanoparticle chains or deposited metallic nanobars introduces a scalable approach for charge injection to adjacent semiconductor thin films, thus facilitating cost-effective photodetection [Sarkar et al., Adv. Func. Mat., 2021, 2011099]. The fusion of soft-lithography with template-assisted self-assembly further enhances large-scale bottom-up strategies, providing a cost-efficient printing of plasmonic metasurfaces for superior charge transfer and amplified the photocatalytic processes [Sarkar et al., Adv. Func. Mat., 2021, 2105054]. Complementing these studies, introducing a novel interconnected metal-semiconductor grating design showcases enhanced current modulation, allowing for efficient photosensor development by leveraging plasmon-mediated hot electrons [Sarkar et al., Adv. Func. Mat.,2023, 2210172]. Thus, our unified approach to bottom-up techniques in plasmonic charge transfer advances the field and promises efficient and scalable solutions for miniaturized optoelectronic devices.

CPP 40.4 Thu 11:30 MA 141

Electrochemistry at the surface of electrically connected plasmonic resonators — •Paul Mörk[1], Amro Sweedan[2], Muhammad Y. Bashouti[2], Bert Hecht[1], and Thorsten Feichtner[1] — [1]Nano-Optics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Ilse-Katz Institute for Nanoscale Science & Technology, Ben-Gurion University of Negrev, POB 653, Beer-Sheba Campus, Building 51, 8410501, Israel

Electrochemical reactions can be enhanced by catalytic processes at gold surfaces. Nanostructuring can lead to plasmonic resonances in the visible wavelength which may be used for photon routing, local heating or hot electron generation. This way it is possible to tailor the properties of gold for specific photo-electrochemical processes.

Here we discuss the use of electrically connected double-wire gratings as an effective plasmonic platform [1]. The gratings are fabricated from monocrystalline gold platelets via focused ion beam milling. We observe the electrochemical oxidation and reduction of these gold double-wire gratings at ambient conditions when applying voltages up to 10 V over gaps of 20 nm in width. We further show the dimerization of 4-aminothiophenol under continuous irradiation and the reverse reaction in presence of an applied voltage. Finally, we show a first implementation of the gratings as electrodes within nanofluidic channels for future applications as electrochemical cell.

[1] Sweedan, Amro, et al., arXiv preprint arXiv:2308.01395 (2023).

CPP 40.5 Thu 11:45 MA 141

Atomic scale plasmonic catalysis — •Yicui Kang and Emiliano Cortés — Nanoinstitute Munich, LMU Muenchen, Germany

In the realm of plasmonic catalytic systems, much attention has been devoted to the plasmon-derived mechanisms1, yet the influence of nanoparticles (NPs) crystal facets has been sparsely investigated. In this work2, we study the plasmon-assisted electrocatalytic CO2RR using three different shapes of plasmonic Au nanocube (NC), rhombic dodecahedron (RD) and octahedron (OC) - with different exposed facets: {100}, {110} and {111}, respectively. Upon plasmon excitation, Au OCs and NCs exhibited nearly a doubling in the FE(CO) compared to non-illuminated response. In contrast, RDs showed nearly the same performance in dark or light conditions. Electromagnetic modeling showed higher electric field (EF) enhancement on OCs and NCs on the edges and corners, which in some degree contributes to the enhancement of CO production3. Large-scale atomistic simulations of the electronic structure revealed higher hot carrier abundance on OCs and NCs compared to RDs. Abundant hot carriers on edges facilitate molecular activation, leading to enhanced selectivity and activity. This observation is further supported by plasmon-assisted HER experiments. Our findings highlight the dominance of low coordinated sites over facets in plasmonic catalytic processes, providing valuable insights for designing more efficient catalysts for energy conversion and carbon neutralization. Ref1. ACS Energy Letters 7.2 (2022): 778-815 Ref2. Crystal Facet Effect in Plasmonic Catalysis. Revision (2023) Ref3. Angew.Chem.Int.Ed.61.44 (2022): e202212640

CPP 40.6 Thu 12:00 MA 141

Translucent aerogel supports for photocatalysis — •David Kiwic, Fabian Matter, and Markus Niederberger — Laboratory for Multifunctional Materials, Department of Materials, ETH Zürich, Vladimir-Prelog-Weg 5, 8093 Zürich, Switzerland

Efficient light absorption is a key part of designing a photocatalytic process. In catalysts light can be scattered or absorbed before reaching the intended absorption site. Metal oxide aerogel supports minimize these light transport losses and their open porous structure enables sufficient gas transport to the active sites. These photocatalysts can be fabricated by synthesizing selected metal oxide nanoparticles, cogelling them with plasmonic nanoparticles, shaping them into granules via extrusion and subsequent super-critical drying. Pd on ZrO2 is known in the field of conventional thermal catalysis to be highly active for CO2 reduction, a key reaction for the decarbonization of our economy. Additionally, Pd nanoparticles strongly absorb visible light and shall be investigated for their photocatalytic activity. Aerogel granules were produced and catalytically tested in thermal and photothermal catalysis with a custom-built reactor setup that enables simultaneous heating and illumination of the granules in the fixed bed. The space time yield of the main product CO was increased manifold by illumination with two white LEDs, demonstrating the great potential of translucent aerogels as support materials for photocatalysis.

CPP 40.7 Thu 12:15 MA 141

Plasmonically generated low-energy electrons: the decomposition of DNA nucleobases derivatives study case — •Sergio Kogikoski Junior[1], Janka Kopyra[2], Janusz Rak[3], and Ilko Bald[1] — [1]Institute of Chemistry, University of Potsdam, Germany — [2]Faculty of Sciences, Siedlce University of Natural Sciences and Humanities, Poland — [3]Faculty of Chemistry, University of Gdansk, Poland

One outcome of the excitation of plasmonic nanoparticles is the generation of low-energy charge carriers ($E < 0.5$ eV). Our group showed that such charge carriers could drive chemical reactions at the interface of Au and Ag nanoparticles using different probe molecules, such as bromoadenine. However, it is still unclear how such molecule activation happens and what the energy of these carriers is. Herein, we used modified DNA nucleobases as probes to understand the role of the support metal and the low-energy electrons generated. The activation mechanisms to drive reactions using low-energy electrons are already well-studied in the gas phase of such molecules, providing a suitable theoretical background. SERS was used to obtain the molecular fingerprint of the system during irradiation. Our results show that irradiated AgNPs can decompose uracil and adenine derivatives, possibly related to the higher amount and energy of the generated hot electrons. Also, adenines are readily decomposed, even though studies in the gas phase show that both molecules decompose. The results show an energy landscape of plasmonically generated hot charges and its relation to probe molecule structure.

CPP 40.8 Thu 12:30 MA 141

Light-driven hydrogen evolution at copper surfaces: machine-learning accelerated nonadiabatic dynamics light the way — •Alexander Spears, Wojciech Stark, and Reinhard J. Maurer — University of Warwick, Coventry, United Kingdom

Light-induced ultrafast dynamics entail the energy transfer between light, electrons, and phonons at interfaces. Whether or not this energy transfer can be harnessed to selectively drive photocatalytic processes remains an open question. Machine-learning interatomic potentials based on electronic structure theory enable the efficient statistical sampling of chemical dynamics at metal surfaces. Molecular dynamics with electronic friction (MDEF) provide a fully anharmonic mixed quantum-classical description of electron-phonon coupling, whereby electronic friction is usually approximated with a free electron gas model. This method has previously been used to model state-resolved scattering experiments or in the calculation of vibrational lifetimes after femtosecond laser pulses, though its validity has yet to be fully assessed. Herein, we present ML-enabled MDEF simulations of thermal and light-driven hydrogen recombination and desorption probabilities from various copper surface facets. We compare results based on electronic friction based on first-order response theory and the free electron gas model and analyse the ability of different approximations to accurately describe the non-adiabatic energy transfer between the surface and adsorbates. Our approach also allows us to study the role of quantum nuclear effects on the dynamics of light-driven associative desorption.

CPP 40.9 Thu 12:45 MA 141

Strong Light-Matter Interaction to Control Plasmonic Catalysis — •Christian Schäfer, Jakub Fojt, and Paul Erhart — Department of Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden

Optically excited nanoplasmonic particles are efficient catalysts, for which an intricate interplay of internal carrier generation and heat drives the reactions of molecules in close proximity. Here, we establish a connection between optical strong coupling between resonator structures and the nanoplasmonic plus molecule system to non-intrusively control the optical excitation energy. Based on a theoretical description from first principles (1,2,3), we demonstrate that this non-intrusive control can be used to optimize carrier injection into the molecule and thus improves plasmonic catalysis. We discuss current limitations, future development, and the prospects of strong coupling modified plasmonic catalysis.

[1] C. Schäfer and G. Johansson, PRL 128, 156402 (2022). [2] C. Schäfer, J. Phys. Chem. Lett. 2022, 13, 6905-6911. [3] C. Schäfer, J. Fojt, P. Erhart, in progress (2024).

CPP 40.10 Thu 13:00 MA 141

Anisotropic core-shell particles in the strong coupling regime — •Mathis Noell and Carsten Henkel — Universität Potsdam, Institut für Physik und Astronomie, Germany

Plasmonic particles coated with resonant organic absorbers (e.g., J-aggregates) provide a versatile platform to observe strong coupling. Calculations using Mie theory result, however, in the prediction of a "spurious" unobserved absorption peak between the upper and lower polariton [1]. The spurious resonance was previously thought to be caused by a negative value of the shell permittivity [2]. Alternatively, recent literature has shown that power broadening of the exciton transition efficiently suppresses the spurious resonance [3]. We demonstrate, using a modified Tavis-Cummings model, that the assumption of an isotropic shell material leads to the excitation of plasmonic dark modes (PDM) by an external field and, consequently, to an absorption line located between the upper and lower polariton. Anisotropic transition dipoles with a fixed orientation relative to the particle surface can fully suppress the coupling between the PDM and the illumination field.

[1] T. Uwada, R. Toyota, H. Masuhara, and T. Asahi, J. Phys. Chem. C 111 (2007) 1549.

[2] T. J. Antosiewicz, S. P. Apell, and T. Shegai, ACS Photonics 1 (2014) 454.

[3] F. Stete, W. Koopman, G. Kewes, C. Henkel, O. Benson, and M. Bargheer ACS Photonics 10 (2023) 2511.

CPP 41: Focus Session: Wetting on Adaptive Substrates II (joint session CPP/DY/O)

The focus session aims to discuss recent developments in the wetting dynamics of adaptive, deformable, and switchable surfaces.

Time: Thursday 11:30–13:00 Location: H 0107

Invited Talk CPP 41.1 Thu 11:30 H 0107

A multi-scale approach to characterize wetting within a porous medium — •Maja Rücker[1], Ryan T. Armstrong[2], Chenhao Sun[3], Peyman Mostaghimi[2], Steffen Berg[4,5], Paul Luckham[5], Apostolos Georgiadis[4,5], and James E. McClure[6] — [1]Eindhoven University of Technology, Eindhoven, NL — [2]University of New South Wales, Sydney, Australia — [3]China University of Petroleum, Beijing, China — [4]Shell Global Solutions International B.V., Amsterdam, NL — [5]Imperial College London, London, UK — [6]Virginia Tech, Arlington, VA, USA

Considering a porous medium with two fluids in it, the fluid flow and distribution will depend on the wetting characteristic of the system. Recent developments in imaging techniques, such as micro-computed tomography and atomic force microscopy, alongside advances in computational modelling allowed for new concepts linking macroscopic wetting responses to the fundamental microscopic wetting definitions to emerge. We present an approach to upscale wetting parameters building upon energetic and geometric considerations and accounting for the various mechanisms related to wetting, manifesting at those different length scales. Starting from fluid-solid interactions, through the motion of three-phase contact lines to the evolution of fluid configurations in the porous medium, we show experimental observation on a coherent set of fluid/fluid/solid systems and discuss those in relation to the proposed upscaling concept. We will highlight the remaining questions for the characterization of wetting in the context of multiphase flow in porous media and point out future research directions.

CPP 41.2 Thu 12:00 H 0107

Soft Wetting Transition — •Christopher Henkel[1], Vincent Bertin[2], Jacco H. Snoeijer[2], and Uwe Thiele[1,3] — [1]Institut für Theoretische Physik, Universität Münster, Germany — [2]Physics of Fluids Group, Faculty of Science and Technology, Mesa+ Institute, University of Twente, The Netherlands — [3]Center for Nonlinear Science (CeNoS), Universität Münster, Germany

We investigate the forced receding dynamics of a three-phase contact line on a viscoelastic substrate. Thereby, we use the Landau-Levich (or dip-coating) geometry, where a solid viscoelastic plate is dragged out of a liquid bath. We employ a mesoscopic hydrodynamic model in long-wave approximation, i.e. valid at small contact angle and plate inclination. The elastic response of the substrate follows the Winkler foundation with a Kelvin-Voigt relaxation. In particular, we investigate how the shape and stability of the meniscus change with the plate velocity and the viscoelastic substrate properties. Finally we compare numeric results with asymptotic analytic calculations.

CPP 41.3 Thu 12:15 H 0107

Demixing around liquid droplets — •Khalil Remini and Ralf Seemann — Experimental Physics, Saarland University, Saarbrücken, Germany

Equilibrium polystyrene droplets are explored sitting on soft solid substrates. The soft solid substrates consist of commercial polydimethylsiloxane (PDMS) elastomer kits with elastic module varying across several orders of magnitude (3-1200 kPa). Inspecting the there-phase contact line of the droplets on a nanoscopic length scale by atomic force microscopy, i.e. on a length scale well below the elasto-capillary length, where capillary forces are higher than the elastic force of the substrate, we find that the ridge formed by the elastic substrate around the droplet is similar to that of a liquid. Material contrasts confirm a liquid ring surrounding the droplets at the three-phase contact line, as a result from stress induced demixing of non-crosslinked PDMS molecules from the PDMS elastomer matrix. This liquid ring extends for softer PDMS elastomers having a larger content of non-crosslinked molecules, but it is present also for the stiffer elastomers. So, the Neumann construction at the three-phase contact line is valid for all tested PDMS elastomers when measuring locally with sufficient resolution.

CPP 41.4 Thu 12:30 H 0107

Chemical reactions confined in liquid films: dynamics and stability — •Tilman Richter[1], Paolo Malgaretti[1], Thomas M. Koller[2], and Jens Harting[1] — [1]Forschungszentrum Jülich GmbH, Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien (IEK-11), Cauerstr. 1, 91058 Erlangen, Germany — [2]Institute of Advanced Optical Technologies - Thermophysical Properties (AOT-TP), Department of Chemical and Biological Engineering (CBI) and Erlangen Graduate School in Advanced Optical Technologies (SAOT), Friedrich-Alexander-Universit Erlangen-Nuernberg (FAU), Paul-Gordan-Straße 8, 91052 Erlangen, Germany

In catalytic reactions occurring within small liquid droplets or thin liquid films, the yield significantly differs from that in bulk reactions. This variance is primarily due to the fluid interface's substantial surface-to-volume ratio. The fluid interface initiates several phenomena, such as increased surface diffusion, Marangoni flows, and more effective surface interactions, which can boost yield substantially. We develop a theoretical model that demonstrates that the uneven distribution of reactants and products, caused by chemical reactions, can induce Marangoni flows. These flows then alter the spatial distribution of the catalyst. This complex interaction offers novel methods for either inhibiting or promoting the rupture of thin films, as well as for modifying the shape of small droplets.

CPP 41.5 Thu 12:45 H 0107

Dynamic vesicles on adaptive surfaces — •Lucia Wesenberg, Ben Rasmus Sprötge, Kai-Uwe Hollborn, and Marcus Müller — Institut für theoretische Physik, Georg-August-Universität Göttingen

Vesicles on substrates play a fundamental role in numerous biological transport processes, such as the neurotransmitter release at the synapse, transport vesicles in cells, or the nutrient intake of trees by large vesicles. For all of these processes the adaptive adhesion of the vesicles to a biological substrate is crucial. Furthermore, it is interesting to compare how these adaptive processes differ from wetting of liquid droplets as their shapes seem similar, however, one is governed by bending rigidity and the other by tension.

Here, we study the equilibrium shapes of vesicles as well as their dynamic adaptation to a changing substrate. Our simulations show the significant impact of buoyancy on the vesicle shape, especially in the contact zone. We are able to construct an adsorption diagram summarizing the metastable region of upward buoyant adsorbed vesicles. Further, we study permeable vesicles, adapting dynamically to substrates with a constant adhesion potential with periodically modulated strength or a steplike potential with a given velocity. A step in the potential allows the steering of vesicles, while periodic switching enables controlled vesicle substrate contact. Thus, both cases prove to be an effective control mechanism for biological transport of vesicles.

CPP 42: Gels, Polymer Networks and Elastomers III

Time: Thursday 15:00–16:45 Location: H 0106

CPP 42.1 Thu 15:00 H 0106

SAXS analysis of electrically controlled drug release hydrogels for diabetes treatment — •Yining Sun[1], Clement Blanchet[2], and Michael Gradzielski[1] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Institut für Chemie, Technische Universität Berlin, Straße des 17. Juni 124, D-10623 Berlin, Germany — [2]European Molecular Biology Laboratory, Hamburg Outstation, Notkestrasse 85, 22603 Hamburg, Germany

Herein, we present the fabrication of conductive hydrogels that were prepared using quaternized chitosan grafted with polyaniline (QCSPA), polyvinyl alcohol, and boronic acid. This hydrogel was dynamically crosslinked by boronate esters between alcohol and boronic acid and ionic interactions between chitosan and boronic acid. The modified QCSPA endows the good bulk conductivity of the hydrogel. We studied the crosslinking of this hydrogel by rheology and small angle scattering (SAXS and SANS), especially the effect of the QCSPA content. Besides, the passive diffusion and electro-triggered insulin release behavior are also studied by SAXS, to observe the relations between hydrogel structure and insulin release kinetics. The obtained results underline the importance of mesh size in the release procedure, which can be designed by varying hydrogel components. The resulting hydrogel demonstrates electrically triggered insulin release, aiming at localized and on-demand therapeutic delivery. The system shows high current tolerance, high drug loading capacity, and is effective in vitro drug release, which suggests a new method to advance diabetes treatment.

CPP 42.2 Thu 15:15 H 0106

Striking a Delicate Balance: Mussel-Inspired P(NIPAM-co-Dopamine Methacrylamide) Microgels with Improved Mechanical and Adhesive Properties — •Sandra Forg and Regine von Klitzing — Soft Matter at Interfaces (SMI), Institute for Physics of Condensed Matter, Technical University of Darmstadt, Darmstadt, Germany

Marine organisms such as mussels have captured the interest of the scientific community due to their exceptional under-water adhesive capabilities and mechanical properties. The catechol-based dopamine methacrylamide (DMA) can serve as a synthetic replacement to mimic the mussel's properties. It has the ability to cross-link polymers.

When DMA is combined with the versatile microgels, systems that exhibit stimuli-responsiveness, mechanical durability, self-healing capabilities, and high surface adhesion can be created. This study offers a thorough exploration of mussel-inspired poly(N-isopropylacrylamide) (PNIPAM) microgels co-polymerised with DMA. These P(NIPAM-co-DMA) microgels adsorbed at the solid surface are characterised by atomic force microscopy (AFM). Their mechanical properties, as well as their adhesive properties were examined by using different probe shapes and sizes (tips vs. colloidal probes). One challenge in the design of mussel-inspired materials is optimising its adhesion while preserving toughness. DMA's cross-linking ability could counteract the adhesion of microgels to surfaces, adding complexity to the development process.

This research provides valuable insights into these novel microgels and establishes a robust foundation for potential future applications.

CPP 42.3 Thu 15:30 H 0106

Exploring Hydration Mechanisms in Poly(N-isobutyramide) and its Isomer, Poly(N-isopropylacrylamide) — •Morgan P. Le Dû[1], Julija Reitenbach[1], David P. Kosbahn[1], Lukas V. Spanier[1], Cristiane Henschel[2], André Laschewsky[2], Robert Cubitt[3], Christine M. Papadakis[4], and Peter Müller-Buschbaum[1,5] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Fraunhofer IAP, 14476 Potsdam, Germany — [3]ILL, 38000 Grenoble, France — [4]TUM School of Natural Sciences, Soft Matter Physics, 85748 Garching, Germany — [5]MLZ, TUM, 85748 Garching, Germany

Thermo-responsive polymers hold a prominent position due to the easy access to the temperature parameter. This study investigates Poly(N-isobutyramide) (PNVIBAM) and compares it with its structural isomer, Poly(N-isopropylacrylamide) (PNIPAM). PNVIBAM exhibits a slightly higher LCST than PNIPAM in aqueous solutions. This makes PNVIBAM particularly well-suited for applications requiring temperature sensitivity to the human body. We investigate the swelling behavior of both polymers when used as thin films and exposed to high humidity conditions. Swelling characteristics are obtained via spectral reflectance and in situ FTIR is used to explore the hy- dration mechanisms in both polymers. Neutron reflectometry (NR) offers crucial insights into their equilibrium swollen state and water content. This research contributes to the understanding of PNVIBAM and PNIPAM properties regarding their hydrophilic behaviour.

CPP 42.4 Thu 15:45 H 0106

Restricted mobility of Ni nanorods in agarose hydrogels — •Nils Boussard and Andreas Tschöpe — Universität des Saarlandes, Experimentalphysik, Campus E2 6, 66123 Saarbrücken

The three-dimensionally linked polymer network in an agarose hydrogel has large pore sizes in a range comparable to the typical length of Ni nanorods ($\langle L \rangle = 100 - 600nm$). The liquid that fills the interstices of the network provides a medium for the movement of embedded particles and the aim of the present study was to investigate how the rotational motion of the magnetic nanorods in agarose hydrogels (0.3-1.0 wt.%) is constrained by the scaffold. To quantify the microstructure of the agarose hydrogels a correlation length ξ was obtained from spectrophotometric turbidity measurements. Due to a magnetic field during gel formation, the ferromagnetic nanorods could be aligned in parallel for the initial state and after switching off this field, the rods relaxed into a stationary orientation distribution. This state could be quantified via optical transmission measurements by an alignment parameter which correlated qualitatively with the ratio $\langle L \rangle / \xi$. For the combinations of nanorod length and agarose concentration of this study, the Ni nanorods showed the transition from nearly free mobility to fixation and a quantitative model was derived by adapting the Edwards tube model. The topological constraint on the rotational motion of the nanorods was approximated by a confining tube with a diameter proportional to the correlation length.

CPP 42.5 Thu 16:00 H 0106

Deformation-Induced Structure and Temperature Evolution of Natural Rubber — •Eric Euchler[1], Konrad Schneider[1], Anna Katharina Sambale[1], Matthias Schwartzkopf[2], and Sven Wiessner[1,3] — [1]Leibniz-Institut für Polymerforschung, Dresden, Germany — [2]Deutsches Elektronen Synchrotron DESY, Hamburg Germany — [3]TUD Dresden University of Technology, Dresden, Germany

Natural Rubber (NR) vulcanizates show deformation-induced structure evolution, e.g. crystallization, explaining the outstanding mechanical performance in comparison to other elastomers. In this study, combined in situ experiments were realized by synchronizing wide-angle X-ray scattering (WAXS) and infrared (IR) thermography with the mechanical deformation of NR vulcanizates. Owing to the coupled methods, a unique database provides new insights into the mechanical behavior of NR, for example: (i) deformation-induced crystallization is primarily controlled by the mechanical stress; (ii) IR thermography allows to follow crystallization as a function of deformation; (iii) the onset of crystallization causes a rapid increase in temperature, however, only a slight increase in stress; (iv) deformation-induced crystallization shows a saturation plateau, which hardly changes with ongoing deformation; (v) surface temperatures show a certain fluctuation that may indicate a non-uniform crystallite distribution.

CPP 42.6 Thu 16:15 H 0106

Mechanical and rheological properties at the surface of amphiphilic polymer conetworks — •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 mechanics and rheology at the surface of amphiphilic polymer conetworks (ACNs). Two four-arm star-shaped polymer building blocks made up of tetra-poly(ethylene glycol) and tetra-poly(ϵ-caprolactone) form a 3-dimensional amphiphilic network, that serves as a model system for this study. First, the correlation between different synthesis strategies for gel films and their resulting properties will be described. Secondly, the effect of solvents of different polarity on the swelling ability will be presented on different length scales. For this purpose, topology and near surface structure are studied with atomic force microscopy (AFM). We also put special emphasis on the determination of mechanical and rheological properties laterally and orthogonally to the gel surface by carrying out dynamic AFM indentation experiments. In order to evaluate heterogeneities, the mechanical and rheological behavior at the surface of the ACNs will be presented on various length scales (nm - μm). The study shows that the synthesis strategy has a strong effect on the gel structure and on nano/microrheological properties.

CPP 42.7 Thu 16:30 H 0106

How chromophore labels shape the structure and dynamics of a peptide hydrogel — •Frederick Heinz[1], Bettina Keller[1], Jonas Proksch[1], Beathe Koksch[1], Robert Schmidt[2], and Michael Gradzielski[2] — [1]Freie Universität Berlin, Berlin, Germany — [2]Technische Universität Berlin, Berlin, Germany

Biocompatible and functionalizable hydrogels have a wide range of (potential) medicinal applications. In contrast to conventional hydrogels formed by interconnected or interlocked polymer chains, self-assembled hydrogels form from small building blocks like short peptide chains. However, the hydrogelation process for these systems, especially those with very low polymer weight percentage (< 1 wt%), is not well understood. This severely hinders the rational design of self-assembled hydrogels. In this study, we demonstrate the impact of an N-terminal chromophore label amino-benzoic acid on the self-assembly and rheology of hydrogel hFF03 (hydrogelating, fibril forming) using molecular dynamics simulations, which self-assembles into α-helical coiled-coils. We find that the chromophore and even its specific regioisomers have a significant influence on the microscopic structure and dynamics of the self-assembled fibril, and on the macroscopic mechanical properties. Furthermore we find that the solvation shell fibrils by itself cannot explain the viscoelasticity of hFF03 hydrogels. Our atomistic model of the hFF03 fibril formation enables a more rational design of these hydrogels. In particular, altering the N-terminal chromophore emerges as a design strategy to tune the mechanic properties of these self-assembled peptide hydrogels.

CPP 43: Wetting, Fluidics and Liquids at Interfaces and Surfaces (joint session CPP/DY)

Time: Thursday 15:00–17:30 Location: H 0107

CPP 43.1 Thu 15:00 H 0107

Dynamic wetting of concentrated granular suspensions — •Reza Azizmalayeri, Peyman Rostami, and Günter K. Auernhammer — Leibniz-Institut für Polymerforschung, Dresden, Germany

Concentrated granular suspensions are employed in a variety of applications in which the contact line dynamics and internal structure of the suspension interact. The process can be characterized using individual particle analysis and average suspension descriptions. There is a markedly high shear rate at the droplet's contact line. This localized shear rate profoundly affects the suspension's non-Newtonian rheological behaviour. Recent researches have affirmed the applicability of hydrodynamic solutions like Cox-Voinov relation to granular suspensions. Despite these efforts, the impact of particles on the overall flow field and microstructure of densely packed granular systems along the contact line remains unexplored. In this study, a configuration consisting of a pinned droplet on a moving substrate is utilized. Using astigmatism particle tracking velocimetry (APTV), we precisely track the 3D motion of tracer particles within the suspension. Near the advancing contact line, we observe distinct behaviours based on the interaction between particles. A concentrated suspension of low interacting particles violates the Cox-Voinov relationship with particle friction becoming a significant factor. Meanwhile, when strong particle interactions are present the suspension exhibits a yield stress behaviour. The receding contact line exhibits a dynamic curvature that undergoes a transient phase before reaching a stationary state. The results of this study are supported by rheology measurements.

CPP 43.2 Thu 15:15 H 0107

How rheology influences the wetting behavior of droplets — •Günter K. Auernhammer[1], Peyman Rostami[1], Reza Azizmalayeri[1], Valentine Comoy[1], and Mathis Fricke[2] — [1]Leibniz Institute of Polymer Research Dresden, Germany — [2]Department of Mathematics, TU Darmstadt, Germany

We study the spreading of viscous and viscoelastic drops on solid substrates with different wettability. In the early stages of spreading, we find that the viscoelastic drop spreads with faster and a different power law than the Newtonian drop (i.e. aqueous glycerine solution) for the same zero shear rate viscosity. We argue that the effect of viscoelasticity is only observable for experimental time scales in the order of the internal relaxation time of the polymer solution or longer times. Near the contact line, the effective viscosity is lower for the viscoelastic drop than for the Newtonian drop. Together with its shear rate dependency, this difference in effective viscosity can explain the different spreading dynamics. We support our experimental findings with a simple perturbation model that qualitatively agrees with our findings. [https://arxiv.org/abs/2308.14515]

CPP 43.3 Thu 15:30 H 0107

Surface Sensitive Fractioning of Microparticles and Microplastics — •Marek Bekir — Institut für Physik und Astronomie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm

Separation of particles of equal size but different surface energies is nowadays a challenging task. With local-light driven diffusioosmosis (local-LDDO) [1] in combination with microfluidic technology [2] we provide a potential tool for separation of such microparticles and microplastics. The local-LDDO is a phenomenon of a photosensitive azobenzene containing surfactant, where under illumination a dynamic exchange of isomers provides a repulsive flow strong enough to elevate particles up to several micrometers from the liquid-glass interface of the microfluidic chamber. In combination of a superimposed lamellar fluid flow the elevation leads to a stronger passive motion along the streamline. We demonstrate that the lift off depends on the size but also on the surface morphology, surface material and surface coating, too, i.e. differently surface modified particles therefore a different motion velocity.[3]

[1] Feldmann, D.; Arya, P.; Molotilin, TY.; Lomadze, N.; Kopyshev, A.; Vinogradova, OI.; Santer, S. Langmuir 2020, 36, 6994-7004.

[2] Sajeesh, P.; Kumar Sen, A. Microfluid Nanofluid 2014, 17, 1-52.

[3] Bekir, M.; Sperling, M.; Vasquez Muñoz, D., Braksch, C.; Böker, A.; Lomadze, N.; Popescu, M. N., Santer, S. Advanced Materials 2023, 35, 2300358.

CPP 43.4 Thu 15:45 H 0107

Curvature-dependent adsorption of surfactants in water nanodroplets: Insights from molecular dynamics — •Fabio Staniscia and Matej Kanduč — Department of Theoretical Physics, Jožef Stefan Institute, Ljubljana SI-1000, Slovenia

Adsorption of surfactants at curved air-water interfaces plays a major role in phenomena involving nanodroplets, such as emulsification, wetting, heterogeneous catalysis, and aerosol chemistry. Once the nanodroplet becomes small enough, its large curvature can influence the adsorption of surfactants, which has not been thoroughly investigated. At this scope we investigate the adsorption of short-chain surfactants inside water nanodroplets using molecular dynamics simulations. We show that the curvature of the droplet interface enhances adsorption and affects other interfacial properties, such as the preferred surfactant orientation. We relate this behavior to curvature-dependent surface tension of water, described by the Tolman length correction. We show that the influence of curvature on adsorption grows exponentially with the size of the hydrophobic tail of the surfactant. Finally, we use our theoretical model to predict the behavior of larger surfactants and of larger droplets.

CPP 43.5 Thu 16:00 H 0107

Interfacial versus confinement effects in the frequency dependent dielectric response of nanoconfined water — •Maximilian Becker and Roland R. Netz — Freie Universität Berlin, Berlin, Germany

We investigate the frequency-dependent dielectric response of water confined between two graphene sheets with force-field and density-functional-theory based molecular dynamics simulations. We highlight the critical role of the volume over which the dielectric response is averaged when measuring the dielectric susceptibility and introduce a system-size-independent decomposition, allowing us to discern interfacial and confinement contributions to the overall dielectric spectrum. Using this, we discuss the molecular origin of the main absorption features of nanoconfined water from the GHz to the THz regime: While intermolecular orientational correlations govern the interfacial and confinement effects on the 30 GHz Debye peak and the static dielectric constant, the 20 THz librational peak undergoes intensity changes which can be attributed to a change in single-molecule motion. When going from bulk to confinement, DFT-MD simulations reveal the emergence of a broad spectroscopic band arising between 1 and 30 THz, a region which is known to probe the dynamics of hydrogen bonds in water. These results are interpreted in the context of the hydrogen bond network at the water-graphene interface and in two-dimensional water layers which sheds light on the intricate behavior of water molecules within confined environments and contributes to a deeper understanding of their dielectric properties.

30 min. break

CPP 43.6 Thu 16:45 H 0107

Improved displacement efficiency in Ganglia size distribution by invasion of complex fluids — Karthik Nuthalapati[1] and •Ralf Seemann[2] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Universität des Saarlandes, Saarbrücken, Germany

It is well-known that the viscoelastic nature of polymer solutions affects the displacement process when used as displacing fluids, for example, in enhanced oil recovery. Nevertheless, the microscopic displacement efficiency within porous media remains elusive. In this study, we experimentally investigated the impact of polymer viscosity and elasticity on the displacement efficiency of silicone oils with different viscosities. As displacing fluids, we explored four types of complex fluids, including a highly viscous Newtonian fluid, a shear-thinning solution with negligible elasticity, an elastic polymer with constant viscosity, and a viscoelastic polymer solution made from a polyelectrolyte within the Ganglia size distribution. As a result, viscoelastic polymers demonstrated improved displacement efficiency in Ganglia size distribution through the invasion of complex fluids.

CPP 43.7 Thu 17:00 H 0107

The Structure of Water Under Confinement in Periodic Mesoporous Organosilicas Investigated by X-Ray Scattering — •Niels Christian Giesselmann[1], Philip Lenz[2,3], Sophia-Marie Meinert[2], Tamás Simon[2], Wonhyuk Jo[1,4], Nele Naomi Striker[1], Michael Fröba[2,3], and Felix Lehmkühler[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]University of Hamburg, Institute of Inorganic and Applied Chemistry, Hamburg, Germany — [3]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany — [4]European XFEL, Schenefeld, Germany

The effect of pore wall chemistry and pore diameter on the structure of confined water was studied by X-ray scattering on water confined in periodic mesoporous organosilicas (PMOs). A shift in the first structure factor peak at $q \approx 1.8$ Å^{-1} reveals a variation in the density of the confined water in dependence of hydrophilicity and pore size. Smaller and more hydrophilic pores induce a lower density in the water. In contrast to bulk water, the pair distribution functions (PDFs) of confined water show a splitting of the second-neighbour peak into either two, in the case of smaller and more hydrophilic pores, or three separate peaks, in larger and more hydrophobic pores. From the running coordination number we conclude that smaller and more hydrophilic confinement leads to a stronger developed tetrahedral network in confined water, while confinement in larger and hydrophobic pores give tetrahedral arrangements that are bulk-like or even less pronounced than in bulk water.

CPP 43.8 Thu 17:15 H 0107

Unveiling the Role of Surface Hydrophobicity and Defects in Heterogeneous Cavitation by Atomistic Simulations — •Philip Loche[1,2], Matej Kanduč[3], Emanuel Schneck[4], and Roland R. Netz[2] — [1]EPFL, Lausanne, Switzerland — [2]FU Berlin — [3]Jožef Stefan Institute, Ljubljana, Slovenia — [4]TU Darmstadt, Darmstadt, Germany

The reduction of pressure in liquids can lead to vaporization and the formation of bubbles, a phenomenon known as cavitation. Cavitation is commonly observed in hydraulic machinery, ship propellers, and even within biological systems. Liquids can sustain enormous negative pressures until reaching their stability limits, at which point cavitation occurs. While classical nucleation theory well explains the energetics of these events, little is known about the dynamics of interfacial bubble formation.

We quantify the kinetics of heterogeneous cavitation using classical nucleation theory and atomistic simulations of self-assembled monolayers at various contact angles under a constant rate protocol. Our focus is on the impact of surface hydrophobicity and defects. We find that increased hydrophobicity leads to a predominance of heterogeneous cavitation at surfaces. Simulations reveal an exponential relationship between the contact angle and the kinetic prefactor, with heightened hydrophobicity significantly reducing this parameter. The balance pressure, where homogeneous and heterogeneous cavitation rates converge, indicates a critical contact angle for switching between these two effects under realistic pressures and volumes.

CPP 44: Complex Fluids, Colloids, Micelles and Vesicles (joint session CPP/DY)

Time: Thursday 15:00–17:45 Location: H 0110

Invited Talk CPP 44.1 Thu 15:00 H 0110

Colloids and the depletion interaction: multi-phase coexistence of colloidal mixtures — •Remco Tuinier — Laboratory of Physical Chemistry, Department of Chemical Engineering and Chemistry & Institute for Complex Molecular Systems, Eindhoven University of Technology, The Netherlands

Colloids are the building blocks of many natural (e.g., clay, milk, blood) and technological (e.g., paint, storage media, cosmetics, shaving foam) systems. The big question underlying related innovations is how can colloidal systems be formulated and designed towards the desired properties? To do this, the forces between the colloidal particles need to be controlled. Adding depletants (non-adsorbing polymers or small colloids) is key to controlling the attractive interactions [1]. This talk provides a detailed exploration of the phase behaviour of complex colloidal mixtures. While hard spheres can undergo a fluid-solid phase transition, anisotropic hard particles such as rods, cuboids, discs or boards exhibit a richer phase behaviour. The addition of depletants to anisotropic colloids gives rise to orientation-dependent attractions resulting in non-trivial phase behaviour. It is demonstrated that such mixtures exhibit a strikingly rich multi-phase coexistence behaviour [2].

[1] H.N.W. Lekkerkerker, R. Tuinier, M. Vis, Colloids and the Depletion Interaction, 2nd edition, Springer, 2024.

[2] J. Opdam, V.F.D. Peters, H.H. Wensink, R. Tuinier, J. Phys. Chem. Lett. 14 (2023) 199-206.

CPP 44.2 Thu 15:30 H 0110

Light-induced manipulation of colloidal particles in a photosensitive polymer-dye system — •Anna López de Guereñu and Svetlana Santer — Room 2.025 University of Potsdam Physics and Astronomy Karl-Liebknecht-Str. 24-25 14476 Potsdam Germany

In this study, we explore the optical and physical properties of a photosensitive surfactant system consisting of mesoporous silica particles in an aqueous solution with a fluorescent dye and an azobenzene-containing surfactant. The latter undergoes reversible photo-isomerization from trans- to cis-configuration upon UV/blue light exposure on a picosecond timescale, offering precise control over particle aggregation. The formation of the dye/surfactant complex adds complexity to the system.

Light-driven diffusioosmosis (LDDO) facilitates remote colloid control, with mesoporous colloids acting as a source or sink for the surfactant, influencing mutual interactions between particles.

The surfactant's isomerization state determines its adsorption affinities, influencing particle interactions. The trans-isomer accumulates in pores and forms a complex with the dye, while the cis-isomer remains outside the pores. Upon irradiation, the cis-surfactant generates a diffusioosmotic flow, causing a repulsion of particles. Wavelength and intensity modulate this process, allowing to control these structures. The dye provides an additional dimension to the system, adding to its complexity due to its influence on the surfactant isomerization and the LDDO process.

CPP 44.3 Thu 15:45 H 0110

Mesoporous silica colloids: surfactant cleaning, wetting and surface diffusion — •Antonio Stocco — Institut Charles Sadron, University of Strasbourg, CNRS, France

We have investigated the use of mesoporous silica colloids to remove cationic surfactants from water. Porous silica colloids diffuse at the surface of water and in the volume, interacting with cationic surfactants that can adsorb inside the pores of these particles. We observed that surfactant adsorption on mesoporous silica depends dramatically not only on the particle pore size but also on specific counterion effects. We measured striking differences both on a macroscopic property of the interface, i.e. surface tension, and also at a single particle level by evaluating the translational diffusion of partially wetted particles at the fluid interface.

CPP 44.4 Thu 16:00 H 0110

Kinetics of phase separation inside complex random porous media — •Rounak Bhattacharyya[1,2] and Bhaskar Sen Gupta[1] — [1]Department of Physics, Vellore Institute of Technology, Vellore, Tamil Nadu, India 632014 — [2]Institute for Theoretical Physics and BioQuant, Heidelberg University, 69120 Heidelberg, Germany

The kinetics of phase separation of segregating fluid mixtures imbibed in porous media is an active field of research due to its great scientific interest and industrial applications. The subject is well understood in the case of ordered pores (e.g., cylindrical pore). But most of the real experimental porous systems are random in nature and are poorly understood. Experimental limitations come from the difficulties in probing the real space geometry using scattering experiments. Also, the theoretical and numerical studies are challenging because of the complex topology of the materials. At this meeting, we will present the findings of our study on the phase separation dynamics of segregating binary fluid mixtures inside random porous materials using large-scale molecular dynamics simulations. Different random porous structures are considered to understand the effect of pore morphology on the coarsening process. We find the existence of two different growth regimes and the crossover is related to the average diameter of random pores. The Porod law and Superuniversality hypothesis are also examined. Finally, the non-equilibrium aging dynamics and the corresponding scaling laws will be discussed for such systems.

30 min. break

CPP 44.5 Thu 16:45 H 0110

Screening Behavior of Nano-Ions in Aqueous Solutions — •Thomas Tilger and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

Due to their special properties, which make them suitable for many applications, the interest in nano ions grew during the last years. They turned out to be promising new materials for e.g. wastewater treatment, separation of nuclear waste and to stabilize foams. Especially for the last application, it is crucial to understand how the interaction between nano ions and the interaction betweeen interfaces in the presence of nano ions can be described.

To directly measure the interaction between well-defined interfaces, colloidal probe atomic force microscopy (CP-AFM) has proven to be a powerful tool. As a model system for nano ions, we chose superchaotropic Keggin ions in aqueous solutions at different concentrations and investigated their influence on the interaction between colloidal silica beads.

It turned out that - despite their large size of approximately one nanometer - the interaction between the silica beads can still be described by the DLVO-theory of electrolyte solutions, consisting of a van der Waals attraction and an electrostatic double layer repulsion. However, the obtained screening lengths exhibit a significant deviation from the ones expected according to the nominal ionic strength of the solutions. The strength of this deviation increases with the concentration of the solutions and might be a hint for an ion aggregation.

CPP 44.6 Thu 17:00 H 0110

Protein cluster formation in protein-polymer mixtures — •Anusha Hiremath, Fajun Zhang, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Germany

Understanding protein cluster formation is crucial for unraveling the mechanisms behind diseases like Alzheimer's and Parkinson's, which are linked to specific protein aggregation. Protein clusters, serving as precursors in protein crystallization [1], are also essential to comprehend the nature of protein aggregation. In this study, static and dynamic light scattering (SLS and DLS) are employed to investigate Bovine Serum Albumin cluster formation driven by depletion interactions [2] in the presence of Polyethylene Glycol (PEG) with varying sizes and concentrations. Using a two-exponential fit model, we illustrate the decreasing diffusion coefficient trend with increasing PEG concentration and size, marking the transition from a dilute to a semi-dilute regime [2]. This decrease in diffusion coefficients suggests an increased attractive potential between proteins, indicating the formation of small clusters. The apparent molecular weight from SLS indicates the formation of protein clusters above a threshold PEG concentration, which decreases with increasing PEG size. Furthermore, we find that larger PEGs accelerate cluster formation. This work demonstrates that the depletion attraction by adding PEG can balance the electrostatic repulsion, leading to the cluster formation in protein solutions.

[1] Zhang, F., J Phys Condens Matter, 29, 443002(2017). [2] Zosel, F. et al., PNAS, 117, 13482(2020).

CPP 44.7 Thu 17:15 H 0110

Phase Behaviour and Structures Induced by Adding Cosurfactant to Nonionic Micelles - Rodlike Assembly of Small Micelles — Robert F. Schmidt[1], Sylvain Prévost[2], Miriam Simon[3], Yeshayahu Talmon[3], and •Michael Gradzielski[1] — [1]Stranski-Laboratorium für Physikalische Chemie, Inst f. Chemie, TU Berlin, Str. des 17. Juni 124, D-10623 Berlin, Germany — [2]ILL, 71 Rue de Martyrs, Grenoble, France — [3]Dep. of Chemical Engineering, Technion, Haifa 3200003, Israel

Addition of cosurfactant is a way to control systematically structure and properties of surfactant formulations. Normally this leads to continuously changing the packing parameter and transforming spherical to wormlike micelles and at higher concentration to bilayers via a first order phase transition. Here we show a completely different self-assembly behaviour seen for a classical nonionic surfactant (Tween 20) and 2-ethylhexylglycerol (EHG) as cosurfactant. Structural characterisation by light and neutron scattering (SANS) and cryo-TEM, shows that elongated assemblies are formed, which are composed of individual micelles that are locally ordered in a cylindrical fashion. A first-order phase transition takes place but only a smaller fraction of amphiphile is initially forming a bilayer structure and complete transformation to bilayers occurs within the single-phase region for EHG concentrations higher than the ones of the phase transition. This very uncommon structural evolution can be rationalised by the particular structure of the amphiphilic molecules involved and this finding extends our common assumptions about surfactant assembly.

CPP 44.8 Thu 17:30 H 0110

Cryo Atom Probe Studies of 5CB, 8CB and Their Mixture — •Kuan Meng, Patrick Stender, Sebastian Eich, and Guido Schmitz — Stuttgart University, Institute for Materials Science, Heisenbergstr. 3, 70569, Stuttgart, Germany

The development of Cryo-FIB enabled studies of various delicate samples of high interest, such as SEI, ferritin and porous borosilicate. Generally, frozen organic materials exhibit complex mass spectra and a high dependence on measurement parameters. Following our earlier measurements on frozen liquids [1], we are studying the evaporation and fragmentation of different liquid crystals. In detail, 5CB (4-Cyano-4'-pentylbiphenyl) and 8CB (4-Cyano-4'-octylbiphenyl) were chosen for investigation due to their relatively simple chemical structure and hydrophobically-induced stability.

Both types of samples, pure 5CB and 8CB, evaporate predominantly as intact molecules, which suits our previous observation in the n-tetradecane study [1]. As a consequence, these two type of molecules can be distinguished even in the mixture, due to their effective mass difference. The dependence of mass spectra on the evaporation conditions and the miscibility of both species will be presented in the talk.

[1] Meng, K., Schwarz, T., Weikum, E., Stender, P., & Schmitz, G. (2022). Frozen n-Tetradecane Investigated by Cryo-Atom Probe Tomography. Microscopy and Microanalysis, 28(4), 1289-1299.

CPP 45: Modeling and Simulation of Soft Matter IV

Time: Thursday 15:00–16:30 Location: H 0111

CPP 45.1 Thu 15:00 H 0111

Multiscale simulations to understand pairing and stacking at the origin of life — •Laurie Stevens[1], Riccardo Martina[2], Alberta Ferrarini[2], and Marialore Sulpizi[1] — [1]Physics Department, Ruhr Universität Bochum, Germany — [2]Chemical Science Department, Universita di Padova, Italy

Our research focus on life's beginnings by examining nucleotide interactions, a critical point in RNA formation. Using Molecular Dynamics, we aim to understand how self-assembly of these components can promote the synthesis of long polynucleotides. However, due to the system's complexity and scale, traditional ab initio methods are too slow for our targeted timescales of several nanoseconds.

To bypass these limitations, we turn to the Machine Learning approach, employing DeepMD. We train neural networks potentials (NNPs) to mimic the intricate behaviours of nucleotides. As a first step we consider a single AMP molecule in water, where we aim to reproduce the complex free energy landscape as function of the relevant degrees of freedom.

The trained NNPs are able to accurately reproduce the solvation structure around the different chemical groups, as well as the conformational changes associated to the torsional angles around the sugar and the phosphate groups.

CPP 45.2 Thu 15:15 H 0111

Microscopic insights on the puzzling saddle-splay elasticity of nematics — •Davide Revignas[1,2] and Alberta Ferrarini[1] — [1]Department of Chemical Sciences, Padua, Italy — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The elasticity of a nematic liquid crystal is commonly understood in terms of the Frank deformation free energy which involves splay (K11), twist (K22) and bend (K33) elastic constants. There exists, however, a fourth term commonly referred to as the saddle-splay deformation mode, which is associated to the elastic constant K24.

Recent experiments on confined chromonic liquid crystals revealed a twisted ground state which has been ascribed to K24 > K22. This would violate one of the Ericksen inequalities for the stability of the nematic uniform state. In general, experimental estimates of K24 are difficult to obtain and only few, sometimes contradictory data are available. Moreover, the estimation of K24 is a challenging task also for microscopic theories of elasticity; indeed, the very possibility of an unambiguous calculation of this quantity starting from a microscopic model has been questioned.

Here we will present the results of the calculation of the full set of elastic constants, including K24, for simple hard rods in the framework of Onsager theory for nematics. Such results enable us to discuss the possible origin of a twisted ground state for this simple model of nematics, in spite of the absence of microscopic chirality.

CPP 45.3 Thu 15:30 H 0111

Scaling Properties of Tree-like Regular Polymeric Fractals — •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

This study compares regular polymeric Vicsek- and T-fractals with dendrimers using theory and simulations. While all structures show exponential growth in the number of monomers and terminal groups, their structural properties differ significantly. Computer simulations are conducted to analyze the scaling properties of these tree-like self-similar polymeric fractals, using the Bond-Fluctuation-Model with the Metropolis method and the parallelized Wang-Landau algorithm. The radius of gyration, scattering intensity, and θ-point of these systems are examined to study the coil-globule transition of the polymeric fractals. A mean field theory is applied to determine the scaling exponent in different solvent conditions, which is found to be in fair agreement with the simulation data. A transition from almost linear chain behavior to a spherical shape is observed, and this can be controlled by the inherent functionality of the building blocks. Consequently, polymeric fractals can serve as an alternative to dendrimers in the category of hyperbranched polymers.

CPP 45.4 Thu 15:45 H 0111

Modeling phenolic (aero)gels: A computational approach — •Hemangi Patel[1], Matthew Addicoat[2], Barbara Milow[1,3], and Ameya Rege[1,4] — [1]German Aerospace Center (DLR), Institute of Materials Research, Department of Aerogels and Aerogel Composites, 51147 Cologne, Germany — [2]Nottingham Trent University New Hall Clifton Campus — [3]Institute of Inorganic Chemistry, University of Cologne, 50939 Cologne, Germany — [4]School of Computer Science and Mathematics, Keele University, Staffordshire, ST 5BG, United Kingdom

Phenolic aerogels, comprising over 90% gaseous volume, exhibit low density, large surface areas, high pore volume, and minimal thermal conductivity. Derived mainly from resorcinol-formaldehyde (RF) polycondensation, these aerogels find diverse applications. The sol-gel chemistry significantly influences their properties, demanding a bottom-up understanding. Although less explored, molecular design holds immense potential to enhance structure-property relations and accelerate aerogel development. This involves optimizing conditions (temperature, pH, precursor concentrations) and employing data-driven approaches. This work illustrates a novel approach to RF gelation design at the molecular level, simulating the reaction chemistry for approximately 50,000 RF monomer molecules within a proposed framework. Characterization includes varying densities, pore wall curvature, voids, pore-size distributions, and surface areas. This strategy aims to propel development of new molecularly-architected aerogel systems by combining experimental optimization and data-driven simulations.

CPP 45.5 Thu 16:00 H 0111

Impact of local structure variations on air flow through porous sheets — •Karin Zojer[1], Ekaterina Baikova[1], Matthias Neumann[2], Phillip Gräfensteiner[2], Peter Leitl[3], Andoni Rodriguez[3], Andre Hilger[4], Ingo Manke[4], Ulrich Hirn[1], and Volker Schmidt[2] — [1]Graz University of Technology, Graz, Austria — [2]Ulm University, Ulm, Germany — [3]bionic surface technologies, Austria — [4]Institute of Materials, Helmholtz Zentrum Berlin, Berlin, Germany

Predicting the rapid transport of gases through inhomogeneous porous layers is difficult because the flow tends to be dominated by a few effective paths, which differ from the most frequently occurring paths of the structure. By looking at the microstructure, is it possible to predict these most effective transport pathways, assuming that all local variations are known? What combination of local structural properties properties favors these pathways? We combine computational fluid dynamics and pore network pore network simulations with a copula-based property-pair dependence analysis to address these questions for air transport through two model materials. These materials are paper sheets, before and after uniaxial compression, whose microstructural variations are fully known from μ-CT 3D imaging. Compression converts large variations in sheet thickness into large variations in density and is therefore expected to localize the air flow and alter the relevant pathways.

CPP 45.6 Thu 16:15 H 0111

Solubility of NaCl in Aqueous Solution using Kirkwood-Buff Integration — •Abhishek Chattopadhyay, Varun Mandalaparthy, and Nico F. A. van der Vegt — Department of Chemistry, Technical University Darmstadt, 64287 Darmstadt

Aqueous electrolyte solutions are ubiquitous in both chemical and biological environments. While molecular simulations are well suited to study these systems, empirical force fields for ion-ion and ion-water interactions are frequently not sufficiently accurate. The aqueous solubility of electrolytes is particularly sensitive to interactions in solution and thus a useful target in model-validation studies. In this work, we used the chemical potential route to calculate the solubility of NaCl using Kirkwood-Buff (KB) integration for the chemical potential of NaCl in the aqueous phase combined with Einstein integration for the solid phase. We consider the full charge Joung-Cheatham ion model combined with SPC/E water as our model system. The effect of ensemble and finite-size corrections applied to the radial distribution functions and KB integrals on the solubility will also be discussed. The KB integration method provides a computationally efficient and accurate route and can be used to compute salt solubility using ion forcefields developed in our research group which incorporate softer ion-water repulsion than the conventional Lennard-Jones potential[1].

[1] M. P. Bernhardt, Y. Nagata, and N. F. A. van der Vegt. J. Phys. Chem. Lett., 13(16):3712-3717, 2022.

CPP 46: Focus Session: Ultrafast Processes in Organic Semiconductors and Perovskites II (joint session O/CPP)

Time: Thursday 15:00–18:00 Location: MA 004

Topical Talk CPP 46.1 Thu 15:00 MA 004

Time-resolved chiroptical probes to track spin & light polarization in solution-processable semiconductors — •Sascha Feldmann — Harvard University, Cambridge, MA, USA

Chiral solution-processable semiconductors based, for example, on small molecules, polymers or halide perovskites offer an exciting new avenue to simultaneously control charge, spin and light using a single material. This could enable efficient spin-optoelectronic devices ranging from displays and holography to detectors, and even applications in quantum information technology.[1] In this talk, I will give an overview of our recent efforts to understand the underlying mechanisms by developing novel time-resolved chiroptical spectroscopy techniques.

By pushing broadband circular dichroism to diffraction-limited spatial and 15 fs time resolution, we create a spin cinematography technique to witness the ultrafast formation of spin domains in halide perovskite films due to local symmetry breaking and spin-momentum locking.[2] In terms of circularly polarized photoluminescence (CPL), I will first explain the fundamentals and artifacts involved in measuring CPL reliably and introduce an open-access methodology and code to do so [3]. I will conclude by showing our most recent development of a transient broadband full Stokes vector polarimetry with unprecedented time and polarization resolution to track the emergence of chiral light emission [to be submitted].

[1] Nature Reviews Materials 8, 365 (2023)
[2] Nature Materials 22, 977 (2023)
[3] Advanced Materials 44, 2302279 (2023)

CPP 46.2 Thu 15:30 MA 004

Nonlinear Pathways for Coherent Control of Lead Halide Perovskite Lattices — •Sebastian F. Maehrlein — Fritz Haber Institute of the Max Planck Society, Berlin

Lead halide perovskites (LHPs) constitute a vast and highly diverse library of emerging semiconductors. So far, to tailor their optoelectronic properties, the material science community mainly focused on changing the static design of the perovskite lattice by tuning the chemical composition or morphology. Meanwhile, the full potential for dynamic phonon-driven ultrafast material control, as successfully applied for oxide perovskites, has rarely been exploited.

I will present a summary of linear and nonlinear, phononic and photonic, excitation pathways to coherently control lattice vibrations with the help of intense THz fields. This comprehensive toolset not only allows to drive also non-IR active modes, but additionally unlocks phonon phase-sensitive lattice trajectory control. In prototype MAPbBr3 and CsPbBr3, we demonstrate coherent control of the octahedral twists [1], which act as structural order parameter and modulate the optical bandgap. Moving to more complex systems, we unveil counterintuitive lattice coherences in mixed 4-cation LHPs, proving the versatility of our method and providing active feedback to the design of novel energy materials.

We acknowledge fruitful collaborations with the groups of X.-Y. Zhu (Columbia U.), T. Kampfrath (FU Berlin), and S. Mathur (U. of Cologne).

[1] Frenzel et al., Sci. Adv.9, eadg3856 (2023)

CPP 46.3 Thu 15:45 MA 004

Confined Excitons in Lead Halide Perovskite Quantum Dots — •Lena Stickel, Anja Barfüsser, Quinten A. Akkerman, and Jochen Feldmann — Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany

In the past years, lead halide perovskite quantum dots (LHP-QDs) have gained massive attention, due to their unique optoelectronic properties.[1] We discuss sphere-like LHP-QDs, which exhibit distinct resonances in their absorption spectra.[2] By comparing experimental data with model calculations based on weak and strong confinement, the origin of these resonances was investigated. Pump-probe experiments show bleaching and induced absorption signals, which we assign to excitonic and biexcitonic transitions.[3] We further use these well-defined excitonic QDs to study the interaction between LHP-QDs and functionalized ligands.

[1] A. Dey et al. ACS Nano 2021, 15, 10775-10981.
[2] Q. A. Akkerman et al. Science 2022, 377, 1406-1412.
[3] A. Barfüßer et al. Nano Lett. 2022, 22, 8810-8817.

CPP 46.4 Thu 16:00 MA 004

Two-Dimensional Electronic Spectroscopy from First Principles — •Jannis Krumland[1,2], Michele Guerrini[1], Antonietta De Sio[1], Christoph Lienau[1], and Caterina Cocchi[1,2] — [1]Carl von Ossietzky Universität Oldenburg, Physics Department and Center for Nanoscale Dynamics (CeNaD), D-26129 Oldenburg, Germany — [2]Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, D-12489 Berlin, Germany

In recent decades, two-dimensional electronic spectroscopy has been established as an experimental tool that can provide unprecedented insight into ultrafast light-matter interaction. Employing three to four concerted laser pulses, this technique is able to map out the third-order polarizability of molecules and extended systems, which contains rich information about nonlinear optical properties as well as vibronic excited-state dynamics following photoexcitation. Here, we present a first-principles approach to the simulation of two-dimensional spectra based on real-time time-dependent density functional theory and Ehrenfest molecular dynamics, applying it to prototypical molecules such as benzene and pyrene [1]. In contrast to other theoretical schemes, our approach does not require any external parameters and thus offers more predictive power. Several numerical techniques are employed to mitigate the computational complexity, making it manageable even for larger systems that are out of reach with other atomistic methods.

[1] J. Krumland et al., arXiv:2308.09062 (2023)

CPP 46.5 Thu 16:15 MA 004

Excited state symmetry breaking and solvation in quadrupolar dyes — •Katrin Winte[1], Somayeh Souri[1], Daniel Lünemann[1], Fulu Zheng[2], Mohamed Madjet[2], Teresa Kraus[3], Elena Mena-Osteritz[3], Peter Bäuerle[3], Sergei Tretiak[4], Antonietta De Sio[1], and Christoph Lienau[1] — [1]Oldenburg University, Germany — [2]Bremen University, Germany — [3]Ulm University, Germany — [4]Los Alamos National Laboratory, USA

Quadrupolar acceptor-donor-acceptor (A-D-A) dyes represent a versatile and chemically tunable class of prototypical molecular systems for exploring photo-induced charge transfer processes. Their optoelectronic properties are governed by an interplay between electronic tunneling between two arms and vibronic coupling to high frequency modes in each arm. In polar solvents, optical excitation results in a pronounced solvatochromism thought to arise from a light-induced charge localization inside the molecule, induced by an interplay between intramolecular charge separation and solvation[1]. So far, both processes could not be distinguished experimentally. Here, we report the first observation of the vibronic-coupling induced nonadiabatic charge separation in A-D-As. By comparing pump-probe and 2DES spectra recorded with 10fs time resolution in polar and nonpolar solvents, we demonstrate coherent vibrational wavepacket motion during the first 100fs that is largely unaffected by solvation. Our results give evidence for a vibronic-coupling induced double-minimum potential energy surface inducing spontaneous symmetry breaking and charge separation after photoexcitation. [1] E. Vauthey, J. Phys. Chem. Lett. 13,2064 (2022).

CPP 46.6 Thu 16:30 MA 004

THz Control of Coherent Phonon Dynamics in Low-Dimensional Hybrid Perovskites — •Joanna M. Urban[1], Marie Cherasse[1], Michael S. Spencer[1], Maximilian Frenzel[1], Charlotte Berrezueta Palacios[2], Gaelle Trippe-Allard[3], Abdelaziz Jouaiti[4], Sylvie Ferlay[4], Emmanuelle Deleporte[3], Stephanie Reich[2], Martin Wolf[1], and Sebastian F. Maehrlein[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Institute of Experimental Physics, Freie Universität Berlin, Germany — [3]Université Paris-Saclay, ENS Paris-Saclay, CentraleSupélec, CNRS UMR 9024, LuMIn, 91190 Gif-sur-Yvette, France — [4]Université de Strasbourg-CNRS, UMR 7140, France

Charge carrier-phonon interaction governs the outstanding optoelectronic properties of hybrid lead halide perovskites (LHPs). Understanding their complex vibrational dynamics is crucial for harnessing their full potential. Recently, we used intense THz pulses to nonlinearly drive octahedral twist modes in 3D LHPs, demonstrating coherent lattice control at ultrafast timescales [1]. Low-dimensional hybrid LHPs combine the intriguing properties of the soft, polar, and anharmonic lattice with quantum confinement effects arising from the reduced dimensionality. We study quasi-2D layered Ruddlesden-Popper perovskites and 1D hybrid perovskite-like metal halides by THz Kerr Effect spectroscopy and analyze the changes of lattice dynamics with dimensionality reduction, towards a better understanding of exciton self-trapping and charge carrier screening.

References: [1] Frenzel et al., Sci. Adv.9, eadg3856 (2023)

CPP 46.7 Thu 16:45 MA 004

Self-Trapped Exciton Emission in Two Families of Antimony and Bismuth Halide Perovskites — •Lukas Gümbel[1], Philip Klement[1], Meng Yang[2], Sangam Chatterjee[1], and Johanna Heine[2] — [1]Institute of Experimental Physics I and Center for Materials Research, JLU Gießen, Germany — [2]Department of Chemistry and Material Sciences Centre, PU Marburg, Germany

Main group metal halide materials are currently explored for a variety of applications including solar cells, but also light emitting devices (LED), lasers, sensing, and photo-catalysis. They promiss less harmful alternatives to the prominent lead halide perovskites. This study investigates the optical properties of antimony and bismuth halide compounds. Temperature-dependent photoluminescence spectroscopy reveals the electron-phonon coupling andyields a Huang-Rhys factor in trhe range of 5 to 22. The broad emission bands and large Stokes shifts suggest self-trapped exciton (STE) emission, linked to an interaction between the photogenerated electron-hole pairs and the lattice. The intricate interplay of factors like ground and excited state distortion, lattice softness, and electron-phonon coupling necessitates deeper understanding. A systematic analysis contributes to establishing the general structure-property relationships for STE emission in such metal halide perovskite-derivate materials. Additionally, the study delves into the diffusion of self-trapped excitons through temporal and spatial resolved photoluminescence, enhancing comprehension of emission processes.

CPP 46.8 Thu 17:00 MA 004

Direct observation of ultrafast lattice distortions during exciton-polaron formation in lead halide perovskite nanocrystals — •Hélène Seiler[1,2], Zahn Daniela[1], Victoria C.A. Taylor[1], Maryna I. Bodnarchuk[3], Yoav W. Windsor[1,4], Maksym V. Kovalenko[3,5], and Ralph Ernstorfer[1,4] — [1]Fritz Haber Institute, Berlin, Germany — [2]Freie Universität Berlin, Berlin, Germany — [3]EMPA, Dübendorf, Switzerland — [4]Technische Universität Berlin, Berlin, Germany — [5]ETHZ, Zürich, Switzerland

We have employed femtosecond electron diffraction (FED) to directly measure the sub-picosecond lattice dynamics of weakly confined CsPbBr3 nanocrystals following above-gap photoexcitation. The data reveal a light-induced structural distortion appearing on a time scale varying between 380 and 1200 fs depending on the excitation fluence. We attribute these dynamics to the effect of exciton-polarons on the lattice and the slower dynamics at high fluences to slower sub-picosecond hot-carrier cooling, which slows down the establishment of the exciton-polaron population. Further analysis and simulations show that the distortion is consistent with motions of the [PbBr3]- octahedral ionic cage, and closest agreement with the data is obtained for Pb-Br bond lengthening.

CPP 46.9 Thu 17:15 MA 004

Structural Dynamics during Excimer Formation in Fluorinated Zinc-Phthalocyanine Thin Films — •Sebastian Hammer[1], Laurenz Kremeyer[1], Tristan Britt[1], Maximilian Rödel[2], 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]CAE (Center of Applied Energy Research) Bayern„ 97074 Würzburg

In molecular solids, the coupling of charge-transfer and Frenkel states facilitated by inter-molecular vibrational modes can lead to the formation of so called excimer states [1]. The formation of these energetically low lying states is accompanied by a significant structural deformation of the local inter-molecular geometry.

In this contribution we examine the dynamics of the structural deformation during the excimer formation in polycrystalline α-zinc-phthalocyanine thin films by means of ultrafast electron diffraction. Our findings show that the geometric relaxation follows a two-step process (300 fs and $\approx$ 15 ps) and the final geometry is stable beyond 300 ps. Tuning the inter-molecular interaction by means of molecular fluorination reveals that the time-scales of the structural relaxation process are critically dependent on the local energetic environment.

Funding from the DFG (Project 490894053) is gratefully acknowledged.

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

CPP 46.10 Thu 17:30 MA 004

Interrelation between excimer dynamics and crystal structure of molecular solids: The case of perylene and perfluorotetracene — •Dominik Muth, Anton Krüger, Sebastian Anhäuser, Daniel Bischof, Gregor Witte, and Marina Gerhard — Department of Physics and Material Sciences Center, Philipps-Universität Marburg, Germany

Excimer formation in organic semiconductors has been known for approximately 70 years. The phenomenon has, however, recently attracted increased interest due to potential applications in the fabrication of organic white light emitting diodes. Gaining insight into the process of excimer formation in molecular solids and controlling the excimer properties via the intermolecular arrangement is therefore of great interest, also from a fundamental point of view.

In this work, we investigate the excimer dynamics in single crystals of two organic semiconductors, i.e. the prototypical material perylene as well as perfluorinated tetracene via time resolved photoluminescence spectroscopy. For both materials, two different polymorphs are studied, providing insight into the influence of the molecular packing on the formation of excimers. Beside the excimer signatures, resolving the dynamics on a picosecond time scale allows us to explore short-lived higher energetic features, which potentially originate from precursor states of excimers. Varying the temperature from 10 to 295 K as well as determining the polarization of the emitted signatures reveals thermal barriers for the population of certain states and the orientation of the underlying transition dipole moments.

CPP 46.11 Thu 17:45 MA 004

Calculation of Diffusion Properties of Molecular Excitons based on Static Optical Spectra — •Chris Rehhagen and Stefan Lochbrunner — University of Rostock, Institute of Physics

The understanding of the mobility of molecular excitons is fundamental for the use of molecular systems in organic solar cells. Especially a small diffusion length is a bottleneck still limiting the efficiency of light harvesting devices. Often, the diffusion constant of molecular excitons is determined by experimental methods observing e.g. exciton-exciton interaction or quenching processes. Additionally, advanced theoretical tools are used for prediction. In both cases, the effort is significant. In this work, we present a method to predict the exciton diffusion constant using static absorption and emission spectra in combination with basic geometric information of the system. Based on Försters theory the diffusion constant can be calculated from the spectral overlap and the electronic coupling. Both properties can be determined from static spectra based on the methods given in the scientific literature. We analyze these methods in detail. Then, the results are compared with experimentally determined diffusion constants in four different PBI-based solid state systems investigated in our group previously, including one-dimensional aggregates, extended nanoparticles and single crystals. In all cases, we find consistency between the experimental results and our prediction.

CPP 47: Wetting, Droplets, and Microfluidics (joint session DY/CPP)

Time: Thursday 15:00–17:45 Location: BH-N 334

CPP 47.1 Thu 15:00 BH-N 334

Structure Formation in Supraparticles Composed of Spherical and Elongated Colloidal Particles — Yashraj M. Wani[1], Melis Yetkin[2], •Kritika Kritika[1,3,4], Michael Howard[5], Hans-Jürgen Butt[2], Michael Kappl[2], and Arash Nikoubashman[1,3,4] — [1]Johannes Gutenberg Universität Mainz — [2]Max-Planck-Institut für Polymerforschung — [3]Leibniz-Institut für Polymerforschung — [4]Technische Universität Dresden — [5]Department of Chemical Engineering Auburn University

In the present work, we use experiments and computer simulations to investigate the formation of supraparticles (SPs) through the evaporation-driven assembly of spherical and elongated colloidal particles (CPs). We systematically explore how different aspect ratios (λ=4,6,11) of the CPs and the drying conditions influence the final morphologies of SPs. In the evaporation-limited regime, where the rate of CP advection is much larger than the rate of CP diffusion, we find a short-ranged orientational ordering of the CPs on the SP surface and isotropic packing in the core. In contrast, simulations in the diffusion-limited regime show a long-ranged orientational ordering of the rods on the SP surface and local nematic ordering in the core. Additionally, we explore SPs fabricated from rod-sphere mixtures, where a thin shell of rods was observed for the slowly dried SPs. In all cases, we also observe that the porosity of the SPs increases with increasing aspect ratio of the elongated CPs.

CPP 47.2 Thu 15:15 BH-N 334

Investigation of nonlinear electrophoresis in microfluidics with alternating voltages — •Robert Epkenhans[1], Ralf Eichhorn[2], Dario Anselmetti[1], and Martina Viefhues[1] — [1]Bielefeld University — [2]Nordita Stockholm

Electrophoresis (EP) is a common phenomenon in microfluidics used for controlled migration of biomolecules like DNA or for size selective migration in gels. In the linear, low-field regime the EP-mobility is dependent only on the particle-zeta and the ambient electrolyte. Yet, recent studies reveled a polynomial velocity increasement for colloid particles exposed to high electric fields above roughly 100 kV/m with the underlying physical mechanisms still under debate.

In our studies, we quantified the nonlinear response in the mobility of charged particles in a microfluidic PDMS-chip as a function of the applied electric field strength. Therefore, we used 1) a superimposition of low DC-fields (0-13 kV/m) and high sinusoidal alternating fields up to 260 kV/m, 2) asymmetric potentials yielding a vanishing time-averaged mean, but non-vanishing higher-order mean value. We present several data sets for the particle velocities with a variation of ionic concentration and types and the respective higher-order electrophoretic mobilities. Our results suggest that nonlinear-EP forces are rather relevant in insultorbased microfluidics instead of dielectrophoresis. This opens new possibilities for particle separation devices, e.g. DNA-molecules, since the up to date data indicates size- and shape-dependent electrophoresis in the nonlinear regime. Concerning these matters, we provide suggestions for future studies on nonlinear electrophoresis.

CPP 47.3 Thu 15:30 BH-N 334

Dynamic density functional theory for drying colloidal suspensions: Hydrodynamic interactions in spherical confinement — •Mayukh Kundu[1], Yashraj M. Wani[2], Kritika Kritika[2,3,4], Arash Nikoubashman[2,3,4], and Michael P. Howard[1] — [1]Department of Chemical Engineering, Auburn University, Auburn, USA — [2]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [3]Leibniz-Institut für Polymerforschung Dresden, Germany — [4]Institut für Theoretische Physik, TU Dresden, Germany

We investigate the role hydrodynamic interactions (HI) play in the evolution of structures in one-component drying colloidal suspensions confined within spherical droplets. We develop a continuum model for the distribution of hard-sphere particles in the droplet based on dynamic density functional theory (DDFT). To compute the particle flux during drying, we employ an accurate free-energy functional based on fundamental measure theory (FMT) in conjunction with pairwise far-field HI described by the Rotne-Prager-Yamakawa (RPY) mobility tensor. To validate the DDFT model, we compare the DDFT predictions with particle-based Brownian dynamics (BD) and multiparticle collision dynamics (MPCD) simulations in selected cases. We also compare our model to DDFT and particle-based models, including only free-draining HI, in order to systematically characterize the effects of HI between particles. Our work illustrates the importance of including HI in models of nonequilibrium self-assembly processes such as drying and demonstrates a systematic way of constructing such models.

CPP 47.4 Thu 15:45 BH-N 334

Numerical study of evaporation-driven particle deposition on a substrate — •Qingguang Xie[1] and Jens Harting[1,2] — [1]Helmholtz-Institut Erlangen-Nürnberg for Renewable Energy (IEK-11), Forschungszentrum Jülich GmbH, Erlangen, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Nürnberg, Germany

Deposition of functional materials on a substrate is a vital process in printing and coating technologies, playing important roles in numerous applications such as photovoltaics, lithium batteries, and electrolysers. The structure of the deposition is crucial for device performance; however, our understanding of the deposition process is still lacking. We conducted numerical studies on the particle deposition process. Initially, we developed a diffusion-dominated evaporation model using a multicomponent lattice Boltzmann method. We validated the applicability of our model by demonstrating agreement in the time evolution of the interface position of an evaporating planar film and a freely floating droplet with analytical predictions. Subsequently, we investigated the deposition of particles on a substrate by drying a colloidal suspension droplet. We explored, both numerically and theoretically, the effect of friction between the particles and the substrate on the deposition pattern. With an increase in friction force, we observed a transition from a dot-like to a ring-like deposit. More recently, we studied the effect of van der Waals force between particles and substrate wettability on the deposition pattern when drying a thin film. We proposed a strategy to achieve highly uniform deposition.

CPP 47.5 Thu 16:00 BH-N 334

Coalescence of biphasic droplets embedded in free-standing smectic A films — •Christoph Klopp[1], Torsten Trittel[2], and Ralf Stannarius[1] — [1]Otto von Guericke Universität Magdeburg, Institut für Physik, ANP — [2]TH Brandenburg, Fachbereich Technik

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. [1-3]. We investigate micrometer-sized flat droplets consisting of an isotropic core surrounded by a nematic rim (biphasic droplets) in freely suspended smectic A liquid-crystal films. In contrast to purely isotropic droplets which are characterized by a sharp edge and no long-range interactions, the nematic rim introduces a continuous film thickness change resulting in long-range mutual attraction of droplets. We show the appearance of a unique structural wall separating the isotropic cores of the droplets during the merging process.

[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] N. S. Shuravin et al., Phys. Rev. E, 99, 062702 (2019)

15 min. break

CPP 47.6 Thu 16:30 BH-N 334

Mutual information as a measure of mixing efficiency in viscous fluids — •Yihong Shi — Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

Because of the kinematic reversibility of the Stokes equation, fluid mixing at the microscale requires an interplay between advection and diffusion. Here we introduce mutual information between particle positions before and after mixing as a measure of mixing efficiency. We demonstrate its application in a Couette flow in an annulus and show that the mixing efficiency depends in a non-trivial way on the time sequence of rotation. We also determine mutual information from Brownian dynamics simulations using data compression algorithms and demonstrate that advanced neural network based compression algorithms can be applied to estimate mutual information to a high accuracy. Our results show that mutual information provides a universal and assumption-free measure of mixing efficiency in microscale flows.

CPP 47.7 Thu 16:45 BH-N 334

Leveraging geometry and catalyst distribution to optimize the yield of catalytic microreactors — •Goncalo Antunes[1], Paolo Malgaretti[1], and Jens Harting[1,2] — [1]Helmholtz-Institut Erlangen-Nürnberg für Erneurbare Energien, Forschungszentrum Jülich, Erlangen, Germany — [2]Department Chemie- und Bioinginieurwesen und Department Physik, Friedrichs-Alexander-Universität Erlangen-Nürnberg, Nürnberg, Germany

We develop a semi-analytical model for transport in heterogeneous catalytic microreactors, where both reactant and product are in the gas phase. Making use of the lubrication and Fick-Jacobs approximations, we reduce the three-dimensional governing equations to an effective one-dimensional set of equations. Our model captures the effect of compressibility, of corrugations in the shape of the reactor, as well as of a non-homogeneous catalytic coating of the reactor walls. We then show how to optimize the output of product by tuning the geometrical and chemical properties of the reactor, such as its length, for which we find an optimum value. We further explore the compressible regime, in which an optimum corrugation height emerges. This height depend on the distribution of catalytic material. Finally, we apply our theory to a model porous material, and find an optimum pore size that maximizes the output of product.

CPP 47.8 Thu 17:00 BH-N 334

Rolle of water accumulation in dynamic friction on hydrophobic surfaces — •Igor Stanković[1], Pierre-Emmanuel Mazeran[2], and Olivier Noel[3] — [1]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, 11080 Belgrade, Serbia — [2]Sorbonne Universites, Universite de Technologie de Compiegne, Laboratoire Roberval, FRE UTC-CNRS 2012, CS 60319, 60203, Compiegne, France — [3]IMMM, UMR CNRS 6283, Le Mans Universite, Avenue O. Messiaen, 72085 Cedex 09, Le Mans, France

The nature of dynamic friction on water molecule-contaminated surfaces is still poorly understood. The capillary phenomena in tribological contact with graphite, a commonly used material, were investigated using circular mode atomic force microscopy and molecular dynamics simulations. Here, we demonstrate that an intuitive paradigm, which asserts that water molecules are squeezed out of hydrophobic contacts, needs to be refined. Consequently, we introduce a mechanism considering a droplet produced within the sliding nanocontact by the accumulation of water adsorbed on the substrate. Our results show that a full slip regime of the droplet sliding on the hydrophobic substrate explains the experimental tribological behaviour.

References 1. O.Noel, P.-E. Mazeran, I.Stanković, ACS Nano 16, 10768-10774 (2022).

CPP 47.9 Thu 17:15 BH-N 334

Active-matter-fueled interfacial microflows — •Kuntal Patel[1,2] and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany — [2]Max-Planck-Institut für Sonnensystemforschung, Göttingen, Germany

Several chemical and biomedical applications require systematic processing of micron-sized fluid samples. To realize this, so-called microfluidic lab-on-a-chip devices with micron-sized channels are widely used. Often, one needs to manipulate interfaces separating immiscible fluids in such channels. The interface separating the two fluid components costs energy, which is quantified by surface tension. Thus, any deformation of a planar fluid interface increases energy.

In our work, we assign one more property to the interface in the form of dipolar forces acting perpendicular to the interface. We name it the *activity* of the interface, and it is achieved by covering the interface with active particles. The notion of activity is inspired by swimming microorganisms. Using lattice-Boltzmann simulations, we discover that the presence of activity affects the stability of the interface. We notice that dipolar forces pointing towards the interface counter the stabilizing effect of surface tension, so that the interface deforms. In contrast, force components pointing away stabilize the planar interface. We demonstrate that one can leverage such activity-induced instability to generate microfluidic droplets and manipulate liquid sheets. In addition, we can also control droplet formation by varying the magnitude of dipolar forces in real time, which can be accomplished using light-sensitive active particles in practice.

CPP 47.10 Thu 17:30 BH-N 334

Extracting oil from an oil and water mixture by using their different wetting properties via the Acoustowetting phenomenon — •Ofer Manor — Technion - Israel Institute of Technology, Haifa, Israel

The free surface of an oil in water emulsion usually catalyzes the formation of a thermodynamically favorable oil film far before the emulsion destabilizes in the bulk of the mixture: We stabilize 170 nm nanoemulsions by surfactants—SDS or Tween 20. The emulsions remain stable for 12 months in closed vessels. However, micron thick oil films appear within minutes on 10 micro-liter sessile drops of the emulsions. We extract the micron-thick oil film off the free surface of the emulsion drops using a traveling 20 MHz-frequency surface acoustic wave (SAW) in the solid.

In our experiments, we place drops of emulsion atop a lithium niobate substrate that supports a traveling SAW therein. Oil films leaks off the emulsion sessile drops 1-20 minutes from the commencement of the experiment, dynamically wetting the solid under acoustic stress—the Acoustowetting phenomenon. The Acoustowetting phenomenon discriminates between the water and oil phases via their wetting properties: The SAW powers the dynamic wetting of the solid by the oil film, extracting oil mass off the emulsion drops, while keeping the higher surface-energy water phase in place. The thickness of the oil film, leaking off the drops, oscillates between 20 to 1 microns and sustains a crystal-like pattern of lateral micron dimensions and submicron thickness of unknown origin in the presence of the SAW.

CPP 48: Members' Assembly

Time: Thursday 18:00–19:00 Location: H 0110

All members of the Chemical and Polymer Physics Division are invited to participate.

CPP 49: Organic Electronics and Photovoltaics IV

Time: Friday 9:30–10:45 Location: H 0107

CPP 49.1 Fri 9:30 H 0107

Interfacial engineering via modifications of the electron blocking layer in PbS quantum dot solar cells — •Huaying Zhong[1], Timo Piecuch[1], Wei Chen[2], and Peter Müller-Buschbaum[1,3] — [1]TUM School of Natural Sciences, Chair for Functional Mateials, 85748 Garching, Germany — [2]SZTU, College of Engineering Physics, Shenzhen 518118, China — [3]TUM, MLZ, 85748 Garching

Colloidal quantum dot solar cells (CQDSC) have received tremendous attention as next generation solar cells. Best performances up to 15% power conversion efficiency (PCE) have been achieved using lead sulfide QDs in a heterojunction cell architecture . PbS CQDs are especially efficient in the infrared region, and thus particular interesting for niche 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 large fraction of long wavelength photons at the EBL/active layer interface , the different interfacial energy-level offsets between EBL and absorber layer via tuning the QDs size of EBL are investigated using ultraviolet photoelectron spectroscopy (UPS) and absorption spectroscopy. Furthermore, the corresponding photovoltaic performances are characterized to demonstrate improved interfacial band alignment.

CPP 49.2 Fri 9:45 H 0107

Phase-field simulations of thermal annealing for all-small molecule organic solar cells — •Yasin Christian Ameslon[1], Olivier Ronsin[2], Christina Harreiss[3], Erdmann Spiecker[4], and Jens Harting[5] — [1]HI ERN, Nürnberg, Germany — [2]HI ERN, Nürnberg, Germany — [3]Nürnberg, Germany — [4]IMN, Erlangen, Germany — [5]HI ERN, Germany

Organic solar cells represent an emerging area in the field of photovoltaic devices. The performance relies upon the Bulk Heterojunction (BHJ) morphology whose final structure is impacted by the drying process and additional post treatment. In this study, we investigate the impact of thermal annealing (TA) on the morphology evolution of the well-studied all small molecules DRCN5T:PC71BM mixture. The objective is to determine the physical processes driving the BHJ morphology evolution. Phase field simulations are used to check the impact of the DRCN5T crystallisation related mechanisms (nucleation, growth, crystals stability, impingement, grain boundary coarsening and Ostwald ripening), of the amorphous-amorphous phase separation (AAPS), and of diffusion limitation on the final morphology. The comparison between the simulation results and the experimental data available from literature leads to following conclusions: The BHJ morphology evolution under TA is mainly due to growth of the largest DRCN5T crystals and dissolution of the smallest unstable crystals. Nucleation, impingement, Ostwald ripening, grain boundary coarsening, AAPS are not significantly active during the TA. Finally, the crystal growth could potentially be diffusion limited.

CPP 49.3 Fri 10:00 H 0107

Static and Dynamic Energetic Disorder in Amorphous Organic Semiconductors via Physics-Inspired Machine Learning — •Ke Chen[1], Karsten Reuter[1], and Johannes T. Margraf[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Bayreuth

Organic semiconductors (OSCs) are attractive for electronic applications due to their low cost and mechanical flexibility. However, the relatively low charge mobility (σ) of OSCs hinders their adoption in many commercial applications. Designing high-σ OSCs is therefore highly desirable. In thin film applications many OSCs form amorphous structures, where the static and dynamic energetic disorder of site-energies is one of crucial factors determining σ. Multiscale simulations based on density functional calculations and kinetic models can be used to analyze the energetic disorder in OSCs, but this is computationally prohibitive for realistic amorphous simulation cells containing thousands of molecules. In this context, machine learning (ML) can drastically accelerate these analyses by providing fast and accurate surrogates to density functional calculations. In this work, we apply our recently reported [1] physics-inspired ML approach to predict energy levels and orbital locations of OSC molecules in large amorphous systems. This opens the door towards the multiscale modeling of realistic amorphous OSCs.

[1] K. Chen *et al.*, Chem. Sci. **14**, 4913 (2023).

CPP 49.4 Fri 10:15 H 0107

On the role of energy level offset and exciton reformation in non-geminate recombination of organic solar cells — •Nurlan Tokmoldin[1], Dieter Neher[2], and Safa Shoaee[1,3] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., 10117 Berlin, Germany — [2]Soft Matter Physics and Optoelectronics, Institute of Physics and Astronomy, University of Potsdam, D-14476 Potsdam-Golm, Germany — [3]Optoelectronics of Disordered Semiconductors, Institute of Physics and Astronomy, University of Potsdam, D-14476 Potsdam-Golm, Germany

The performance of modern organic bulk-heterojunction solar cells relies on a transition from a localised singlet exciton on an acceptor molecule (S1) to a charge-transfer state (CT), followed by CT dissociation into separated charge (CS) carriers. The latter may afterwards either be extracted or recombine by reforming CT. Losses may occur at every stage of the free carrier generation and during their lifetime and proceed via radiative and non-radiative decay of S1 and CT. The S1 reformation efficiency from CT then comes forward as a key parameter characterizing the distribution of losses via the different channels. We employ a rate equation analysis to determine the singlet reformation efficiency for several low-offset organic solar cells and find a good correlation with the S1-CT offsets extracted from temperature-dependent electroluminescence quantum yield measurements. This supports our earlier observations that the energy offset affects the bimolecular recombination coefficient in OPV blends and indicates that exciton reformation may indeed act a channel for non-geminate recombination.

CPP 49.5 Fri 10:30 H 0107

Unveiling the Thermal Expansion Behaviour of Organic Semiconductor Thin Films — •Meike Kuhn[1,2], Christopher R. McNeill[2], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]Material Science and Engineering, Monash University, 20 Research Way, Clayton, Australia

Semiconducting polymers have emerged as a promising material for next-generation solar cells. However, for the optimization and reliability of such devices, understanding the thermal behaviour of the organic semiconductor layer is crucial. The thermal expansion impacts the molecular packing and crystallinity of polymers, influencing the charge transport properties of a material. Mismatches in the thermal expansion coefficients between the active layer and the other solar cell layers can furthermore lead to mechanical stress and device failure. In this study, we use temperature-dependent in-situ GIWAXS and NEXAFS spectroscopy to systematically investigate the thermal behaviour of the widely used semiconducting polymer PDBD-T-2F (PM6). Specifically, we investigate the influence of the temperature on the molecular packing, crystallinity and orientation. Additionally, we study the thermal behaviour of PM6:Y6 blends, which are widely used for high-efficiency organic solar cells, to examine the impact of temperature on OSC active layers.

CPP 50: Focus Session: Wetting on Adaptive Substrates III (joint session CPP/DY/O)

The focus session aims to discuss recent developments in the wetting dynamics of adaptive, deformable, and switchable surfaces.

Time: Friday 9:30–12:45 Location: H 0110

Invited Talk CPP 50.1 Fri 9:30 H 0110

Condensation on soft substrates — •Ambre Bouillant[1,3], Bruno Andreotti[2], and Jacco H. Snoeijer[3] — [1]Laboratoire MSC, CNRS UMR 7057, Université Paris Cité, FR — [2]Laboratoire LPENS, CNRS UMR 8023, Université PSL, FR — [3]Physics of Fluids, Twente Unversity, NL

Vapor molecules can nucleate on cool substrates, provided the surrounding humidity is high enough. Dew formation has been investigated on both rigid (and rough!) solids as well as on liquids. However, how substrate elasticity affects the condensation process remains elusive. In this talk, I will present how water condenses on soft, elastic gels that are smooth at the nanometer scale. We prepare PDMS gels whose softness varies between that of a rigid substrate and an un-crosslinked polymeric liquid.

Although elasticity should be marginal at the nanometric scale at which drops form, we report that the nuclei density is highly sensitive to the substrate softness. Throughout this talk, I will delve into the intricate dynamics of condensation and try to explain some of the intriguing characteristics we have observed. Among these are the influence of softness on nucleation; the sub-diffusive growth of droplets; and the absence of secondary nucleation events (unlike what is classically observed in heterogeneous nucleation). Later, when neighboring drops get closer, they attract each other due to interactions mediated by substrate deformations. Drops then gather into clusters that seem reluctant to coalesce. This ultimately results in the formation of a persistent, ordered, honeycomb-patterned liquid film.

CPP 50.2 Fri 10:00 H 0110

Modelling droplets on substrates with travelling-wave deformations — •Josua Grawitter and Holger Stark — Technische Universität Berlin, Institut für Theoretische Physik, Hardenbergstr. 36, 10623 Berlin, Germany

Motivated by strategies for targeted microfluidic transport of droplets, we investigate how sessile droplets can be steered toward a preferred direction using travelling-wave deformations of the substrate. To perform our numerical study, we develop a formalism to apply the boundary-element method to dynamic wetting. It solves the governing Stokes equations for the fluid flow field inside the droplet that is pushed forward by the deforming substrate.

We find two distinct modes of droplet motion. For small wave speed the droplet surfs with a constant velocity on the wave, while beyond a critical wave speed a periodic wobbling motion occurs, the period of which diverges at the transition. In the related case of a flat substrate with travelling waves in wettability, such an observation is well rationalized by the *nonuniform oscillator* model and the transition described by a SNIPER bifurcation. Here, however, the mean droplet velocity in the wobbling state is proportional to the wave speed at large speed values since the droplet always has to move up and down. To rationalize this behavior, the nonuniform oscillator model has to be extended. Since the critical wave speed of the bifurcation depends on the droplet radius, this dependence can be used to sort droplets by size.

CPP 50.3 Fri 10:15 H 0110

High Voltages Generated by Moving Water Drops — •Stefan Weber[1,2], Pravash Bista[2], Aaron Ratschow[3], and Hans-Jürgen Butt[2] — [1]Institute for Photovoltaics, University of Stuttgart — [2]MPI for Polymer Research, Mainz — [3]Institute for Nano- and Microfluidics, TU Darmstadt

Water drops on insulating, hydrophobic substrates can generate electric potentials of kilovolts upon sliding for a few centimeters. We show that the drop saturation voltage corresponds to an amplified value of the solid-liquid surface potential at the substrate. The amplification is given by the substrate geometry, the drop and substrate dielectric properties and the Debye length within the liquid. Next to enabling an easy and low-cost way to measure surface- and Zeta potentials, the high drop voltages have implications for energy harvesting, droplet microfluidics and electrostatic discharge protection.

CPP 50.4 Fri 10:30 H 0110

Electro(de)wetting with Photoswitches: Control of wetting by electric fields and light — •Billura Shakhayeva and Björn Braunschweig — University of Münster, Institute of Physical Chemistry, 48149 Münster, Germany

Electro-dewetting (EDeW) was introduced as a new method in order to change the wetting properties of surfaces. The underlying mechanism is, however, not fully understood and additional experiments are needed. For that, we have replaced the DTAB surfactants used in the original work [1] by arylazopyrazole triethylammonium bromide (AAP-TB) which is a cationic surfactant that can change the surface tension at the air-water interface to a large extend through E/Z photoisomerization [2]. This offers to fine tune the contact angle during EDeW by E/Z photoisomerization of AAP-TB and we find a further increase in contact angle by $\sim 6^\circ$ when the samples were irradiated by UV light that triggers photoisomerization from the E to the less surface-active Z isomer. Li et al.[1] suggested that surfactants are deposited on the silicon oxide surface through the EDeW process. In order to study the possible deposition of surfactants and the role of a possible prewetting layer outside of the drop and at some distance from the 3-phase contact line we have done sum-frequency generation (SFG) spectroscopy and find that surfactants are deposited even several mm adjacent to the drop and that their structure as well as the structure of the accompanying water layer changes drastically close to the 3-phase contact line. [1] Li et al. Nature, 572, 507-510 (2019) [2] Schnurbus et al. J. Phys. Chem. B 124, 6913 (2020).

CPP 50.5 Fri 10:45 H 0110

Light-Triggered Manipulations of Droplets All in One: Reversible Wetting, Transport, Splitting, and Merging — •Maren Umlandt, Nino Lomadze, and Svetlana Santer — University of Potsdam, Potsdam, Germany

We report on light-triggered droplet manipulation such as reversible wetting, splitting, merging, and transport [1]. The unique feature is that the changes in the wetting properties of anisotropic liquids adsorbed on photo-switchable films can be triggered by application of optical stimuli, which lead to changes in the morphology of the surfaces. The adaptive films consist of an azobenzene-containing surfactant attached to oppositely charged polymer chains. Under exposure to irradiation with light, the azobenzene photo-isomerizes between trans- and cis-states, resulting in changes in surface energy and orientation of surfactant tails in film [2]. The increase in the surface temperature due to absorption of light by the azobenzene groups [3] enables diverse processes of droplet manipulation. Using a moving light spot, we demonstrate the locomotion of the droplet over macroscopic distances. Our findings could lead to the application of a programmable workbench for manipulating and operating an ensemble of droplets.

We thanks for funding DFG and RFBR.

[1] Umlandt, M. et al. ACS Applied Materials & Interfaces 2022 14 (36), 41412-41420 [2] Arya, P. et al. J. Chem. Phys. 2020, 152, 024904 [3] Zakharov, A. V.et al. Phys. Rev. E 2017, 96, 052705

15 min. break

Invited Talk CPP 50.6 Fri 11:15 H 0110

Of Singularities and Controversies: The Soft Wetting Enigma — •Stefan Karpitschka — University of Konstanz

The surface mechanics of soft solids are ubiquitously important in nature and technology. Static and dynamic wetting of soft polymer gels by simple liquids has emerged as an archetypical model system: The singular capillary traction at the edge of a droplet creates a microscale wetting ridge which slows down dramatically the macroscopic dynamics. Capillary, elastic, viscous and osmotic effects all contribute simultaneously in a highly non-linear regime, which has sparked controversial discussions of the underlying theoretical description. In this talk I will present recent measurements on ultra-thin to ultra-soft materials, along with new theoretical and numerical results, scrutinizing sources of non-linear behavior in both statics and dynamics.

CPP 50.7 Fri 11:45 H 0110

Dynamics of Moving Droplets on Lubricated Polymer Brushes — •Rodrique Badr[1], Lukas Hauer[2,3], Doris Vollmer[3], and Friederike Schmid[1] — [1]Johannes Gutenberg University, Mainz — [2]Humboldt-Universität zu Berlin, Berlin — [3]Max Planck Institute for Polymer Research, Mainz

The interaction of liquid droplets with lubricated substrates is rich with interesting physics combining thermodynamics, polymer science, and fluid dynamics, and has the potential for various industrial applications. In this work we focus on the dynamics of droplets moving on lubricated polymer brushes. In previous work, we showed the existence of a cloaking transition where the lubricant covers the surface of the droplet at equilibrium. Here, we investigate the influence of this cloak on the dynamics, in addition to its properties during the dynamical steady state. In addition, we investigate the characteristic of the wetting ridge, as well as the flow of the droplet, and quantify the friction forces felt by the droplet during its motion.

CPP 50.8 Fri 12:00 H 0110

Modeling the growth of biofilms on soft substrates — •Anthony Pietz[1], Karin John[2], and Thiele Uwe[3] — [1]Institute for theoretical physics, University of Münster — [2]Institute for theoretical physics, University of Münster — [3]Research Associate at the CNRS Laboratoire Interdisciplinaire de Physique LIPhy Grenoble - France

We investigate the influence of substrate softness on biofilm growth amending the thin-film model developed by Trinschek et al for rigid solid substrates [1] by the inclusion of a simple description of an elastic substrate [2]. Wettability (described in the mesoscopic model by a wetting energy) is a key factor in the transition between arrested and continuous spreading on rigid substrates [1]. Our focus are changes in the spreading process with changing character of the substrate studied by time simulations of 2d drops/biofilms at fixed surface tension and initial drop volume. We find that with increasing softness from rigid via elastic to liquid-like substrate the spreading velocity of the biofilm decreases at fixed biofilm growth rate and wettability. Further, we discus how these changes depend on wettability and growth rate. In particular, we show that the transition between arrested and continuous spreading is for increasing softness shifted towards larger wettability and larger growth rate.

[1] S. Trinschek, K. John, S. Lecuyer, and U. Thiele, Phys. Rev. Lett. 119, 078003 (2017).

[2] C. Henkel, J. H. Snoeijer, and U. Thiele, Soft Matter 17, 10359 (2021).

CPP 50.9 Fri 12:15 H 0110

Chemically Active Wetting — •Susanne Liese[1], Xueping Zhao[2], Christoph Weber[1], and Frank Jülicher[3] — [1]Faculty of Mathematics, Natural Sciences, and Materials Engineering: Institute of Physics, University of Augsburg, Augsburg, Germany — [2]Department of Mathematical Sciences, University of Nottingham Ningbo China — [3]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Wetting of liquid droplets on passive surfaces is ubiquitous in our daily lives, and the governing physical laws are well-understood. When surfaces become active, however, the governing laws of wetting remain elusive. Here we derive the non-equilibrium thermodynamic theory for active wetting, where the surface is active due to a binding process that is maintained away from equilibrium. We show that active binding fundamentally changes the wetting behavior, leading to steady, non-equilibrium states with droplet shapes reminiscent of a pancake or a mushroom. The origin of such anomalous shapes can be explained by mapping to electrostatics, where pairs of binding sinks and sources correspond to electrostatic dipoles along the triple line. This is an example of a more general analogy, where localized chemical activity gives rise to a multipole field of the chemical potential. The underlying physics is relevant for cells, where droplet-forming proteins can bind to membranes accompanied by the turnover of biological fuels.

CPP 50.10 Fri 12:30 H 0110

Intracellular wetting between biomembranes and liquid-like condensates — •Lukas Hauer[1], Katharina Sprobeck[1], Amir Houshang Bahrami[2,3], and Roland L. Knorr[1,4] — [1]Humboldt Univeristät zu Berlin — [2]Bilkent University, Ankara — [3]MPI-DS, Göttingen — [4]University of Tokyo

Wetting has been recently identified as physiologically important in fundamental cellular processes: phase-separated condensates (e.g., proteins and RNA) form liquid droplets in cells and interact with membranes, e.g., during autophagy in eukaryotic cells or protein storage in plant vacuoles. Upon contact, the droplets can exert wetting forces on the membrane that deforms. This creates a competition of mechanical forces of the membrane elasticity and the droplet capillarity, giving rise to elastocapillary phenomena. In this talk, I will present a minimal model system comprising giant lamellar vesicles (GUVs) filled with aqueous phase-separating polymers(PEG/Dextran). We create liquid-liquid interfaces inside GUVs by osmotic quenches, yielding deformed vesicles with excess membrane area. The excess membrane accumulates at the liquid-liquid interface and assumes differing morphologies, ranging from micro-tubules to sheets, to stomatocytes. We find that the morphology transition depends on the liquid-liquid surface tension. Our results will help to explain resembling in vivo observations during the morphogenesis of protein storage vacuoles in plants.

CPP 51: Complex Fluids and Soft Matter (joint session DY/CPP)

Time: Friday 9:30–12:15 Location: BH-N 243

CPP 51.1 Fri 9:30 BH-N 243

Percolation in Suspensions of Rod-like Colloids under Shear Flow — •Victor Tänzel, Fabian Coupette, and Tanja Schilling — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

Suspensions of electrically conductive fillers are an interesting class of material for applications in energy storage and sensor technology. Their practicality depends on the behavior of the fillers, which is intricate and complex for elongated particles in flow.

We use multi-particle collision dynamics (MPC) to model rod-like particles in shear flow of a hydrodynamic medium. Percolation and conductivity are characterized with regard to the system's properties. MPC also allows us to turn off the hydrodynamic interactions from the solvent, so we can assess their influence.

CPP 51.2 Fri 9:45 BH-N 243

orientational order and topological defects in a dilute solutions of rodlike polymers at low reynolds number — •Leonardo Puggioni[1,2], Stefano Musacchio[1], and Guido Boffetta[1] — [1]Dipartimento di Fisica and INFN, Università degli Studi di Torino, via P. Giuria 1, 10125 Torino, Italy — [2]Instituut-Lorentz, Leiden Institute of Physics, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands

The relationship between the polymer orientation and the chaotic flow, in a dilute solution of rigid rodlike polymers at low Reynolds number, is investigated, by means of direct numerical simulations. It is found that the rods tend to align with the velocity field in order to minimize the friction with the solvent fluid, while regions of rotational disorder are related to strong vorticity gradients, and therefore to the chaotic flow. The "turbulent-like" behavior of the system is therefore associated to the emergence and interaction of topological defects of the mean director field, similarly to active nematic turbulence. The analysis has been carried out both in two and three spatial dimensions.

CPP 51.3 Fri 10:00 BH-N 243

Phase Behaviour of Hard Convex Particles — •Poshika Gandhi and Anja Kuhnhold — Institute of Physics, University of Freiburg, Germany

The shape of a particle has a significant influence on its phase behaviour. A simple uniaxial particle, like a spherocylinder, produces a larger variety of phases as compared to a sphere. From the existence of the biaxial nematic phase to the search for a polar nematic one, simulations of hard particles of different shapes and symmetries continue to invoke interest.

We used Monte Carlo NVT simulations to produce phase diagrams of convex biaxial particles with both chiral and achiral compositions. The effect of particle shape on the phase behaviour and the effect of initial configurations on particles with C_{2v} symmetry was analysed. The results show generalised behaviour across particles of varying shapes and sizes which betters our understanding of the entropic forces in simulations of hard particles.

CPP 51.4 Fri 10:15 BH-N 243

Stochastic rotational dynamics of strongly coupled superparamagnetic particles — •Andrey Kuznetsov[1], Sofia Kantorovich[1], Vladimir Zverev[2], and Ekaterina Elfimova[2] — [1]University of Vienna, Vienna, Austria — [2]Ekaterinburg, Russia

We report a theoretical study of the rotational dynamics of interacting superparamagnetic nanoparticles in time-varying magnetic fields. The research is motivated by an increasing interest in biomedical applications of magnetic nanoparticles (such as cancer hyperthermia or magnetic particle imaging). We consider an ensemble of spherical single-domain particles with a uniaxial crystallographic anisotropy. Particles are uniformly distributed in a 3D space, while their easy axes are either co-aligned or distributed at random. We develop a mean-field approach that allows one to describe the dynamics of the system magnetization under oscillating field of arbitrary frequency and magnitude. To test the validity of the theory, its predictions are compared to Langevin dynamics simulations. It is shown, that if the energy of dipolar interactions is comparable to the energy of thermal fluctuations, the theory works well in wide ranges of particle concentrations and anisotropy constants. However, at lower temperatures the agreement breaks down. In particular, for isotropic nanoparticles our theory predicts a Debye-like susceptibility spectrum with a single relaxation time. In simulations we instead observe an emergence of a uniform band of relaxation times, that broadens with the increase of dipolar coupling parameter.

CPP 51.5 Fri 10:30 BH-N 243

Nonequilibrium evolution in long-range attractive systems: initial state dependence and averaging in simulations and theory — •Johannes Bleibel[1] and Martin Oettel[2] — [1]Fachbereich Physik, Universität Tübingen, Tübingen, Germany — [2]Institut für angewandte Physik, Universität Tübingen, Tübingen, Germany

We investigate the dynamics of the so–called capillary collapse of colloidal particles trapped a fluid interface with 1D Brownian Dynamics (BD) simulations and Dynamical Density Functional Theory (DDFT). Interfacially trapped, micrometer–sized colloidal particles interact via long–ranged capillary attraction. The interaction is formally analogous to screened Newtonian gravity with the capillary length λ as the tuneable screening length. Within intensive studies of the dynamics in 2D, it turned out that radially averaged DDFT only captures the dynamics at initial times and largely deviates from simulation results later on. This discrepancy has been traced to the role of an initially averaged configuration in DDFT[1].

In order to shed light on the precise role of initial fluctuations in the averaging process and subsequent dynamics both in BD simulations and DDFT, we investigate the dynamics of infinitely long rods trapped at a fluid interface and thus study the dynamics of a long–ranged attractive 1D fluid under a temperature quench. We apply several distinct averaging recipes for initial conditions and noise and discuss possible effects of averaging in an alternative description using Power Functional Theory (PFT).

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

15 min. break

CPP 51.6 Fri 11:00 BH-N 243

Towards a standard model of liquid matter — •Alessio Zaccone — University of Milan, Department of Physics, 20133 Milan, Italy — Institute of Theoretical Physics, University of Göttingen, Germany

Our understanding of liquid matter made a leap in 20th century physics thanks to the successful mathematical and numerical development of pair correlation functions, which gave unprecedented insights into the structure of liquids. The same is however not true for the dynamical, mechanical and thermodynamic properties of liquids. The most striking example is the inability of celebrated theories to explain the specific heat of liquids or the propagation of acoustic waves in liquids as they are observed experimentally or in simulations. This of course includes the emergence of rigidity as a function of frequency of mechanical oscillation or as a function of confinement, and the Maxwell interpolation between viscous (Newton) and elastic (Hooke) limits, which has remained largely an empirical assumption in many theories of liquids and supercooled liquids, from generalized hydrodynamics to mode-coupling theory. In my talk I will show that these open issues can be understood mechanistically, and in comparison with experiments, by combining advances from different conceptual frameworks: i) the Instantaneous Normal Modes theory of liquid dynamics, and iii) the nonaffine response theory of liquids and glasses [1-3]. [1] A. Zaccone, "Theory of Disordered Solids", Springer, 2023, [2] A. Zaccone, Phys. Rev. E 108, 044101 (2023), [3] K. Trachenko and A. Zaccone, PNAS 117 (33) 19653-19655 (2020).

CPP 51.7 Fri 11:15 BH-N 243

Dilute gel networks vs. clumpy gels in colloid-polymer mixtures — Matthias Gimperlein and •Michael Schmiedeberg — Inst. für Theor. Phys. 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The formation of gels differs from the behavior observed in other slowly relaxing systems [1,2]. A simple system to explore gelation is a colloid-polymer mixture, where there are complex heterogeneous phases due to the competition of short-ranged repulsions, depletion attractions, and longer-ranged screened Coulomb repulsions.

Here we study the differences of dense clumpy gels and dilute gel networks in terms of dynamics and structure formation. For example, we apply reduction algorithms [3,4] and observe that dilute and dense structures differ in the way structural properties like the typical thickness of the strands emerge. We also analyze the percolation behavior [5] and the formation of pentagonal bipyramids (as in [1]).

Finally we demonstrate that neural networks can be trained to recognize the differences between dilute gel networks and clumpy gels.

[1] H. Tsurusawa and H. Tanaka, Nat. Phys. **19**, 1171 (2023).

[2] M. Schmiedeberg, Nat. Phys. **19**, 1078 (2023).

[3] M. Gimperlein and M. Schmiedeberg, J. Chem. Phys. **154**, 244904 (2021).

[4] J. N. Immink, J. J. Erik Maris, R. F. Capellmann, S. U. Egelhaaf, P. Schurtenberger and J. Stenhammar, Soft Matter **17**, 8354 (2021).

[5] M. Kohl, R.F. Capellmann, M. Laurati, S.U. Egelhaaf, and M. Schmiedeberg, Nat. Comm. **7**, 11817 (2016).

CPP 51.8 Fri 11:30 BH-N 243

Thermofluidic Non-equilibrium assembly of Functional Structures — •Desmond Quinn, Diptabrata Paul, and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Leipzig University, 04103 Leipzig

Assembly in equilibrium is dictated by static energy landscapes. Non-equilibrium assembly on the other hand is driven by fluxes that can be controlled by external energy inputs, enabling reconfigurable structures. The non-equilibrium assembly of colloids was explored here, which was mediated by optically driven heat dissipation. The heat dissipated leads to thermofluidic flows and osmotic pressures that drive the colloidal particle towards the heated regions and lead to the formation of ordered structures.

The mechanisms of assembly were disentangled, and the growth dynamics of the structures was modeled. 3D structures were found to assembly in a matter of a few minutes, and the growth dynamics was found to be dependent on the particle fluxes. Analysis of the structure revealed its crystallinity. The emergent photonic properties of such colloidal crystal structures were investigated. A photonic stopband was observed and fit well with theoretical expectations. Furthermore, the photonic property could be modulated by modulating the assembled structure. This shows that non-equilibrium processes could be useful in assembly of reconfigurable functional materials. The manipulation of bacteria was also explored, which is useful to study bacterial interactions.

CPP 51.9 Fri 11:45 BH-N 243

Analysing seismic waves and velocities including interference effects in granular matter of volcanoes — •Regine Frank[1,2], Marcel van Laaten[3], Birger Lühr[4], and Ulrich Wegeler[3] — [1]College of Biomedical Sciences, Larkin University, Miami, Florida, USA — [2]Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain — [3]Institut für angewandte Geowissenschaften, Friedrich-Schiller-Universitaet Jena — [4]Deutsches GeoforschungsZentrum GFZ, Helmholtz-Zentrum Potsdam

We present self consistent diagrammatic transport theory and numerical solutions for the analysis of seismic waves and velocities including interference effects in granular matter of volcanoes. We introduce weighted essentially non-oscillatory solvers (WENO) which are suitable to treat extreme non-linear properties and rogue waves. We compare our numerical results to recent experiments and several other theoretical models.

[1] A. Lubatsch, R. Frank, Phys. Rev. Research 2, 013324 (2020) [2] C. Sens-Schönfelder, U. Wegler, Geophys. Res. Lett., v. 33, no. 21, L21302 (2006) [3] U. Wegler, B.-G. Lühr, R. Snieder, A. Ratdomopurbo, Geophys. Res. Lett., v. 33, L09303 (2006) [4] C. Friedrich, U. Wegler, Geophys. Res. Lett., v. 32, L14312, (2005)

CPP 51.10 Fri 12:00 BH-N 243

Optimal low-resolution representations as a probe of a system's emergent features — •Raffaello Potestio — University of Trento, Trento, Italy

Gathering data from computer simulations of soft and biological matter systems is becoming increasingly easy as our available computational power keeps growing. While hoarding data is thus "easy", making sense of them is a fully different story. Here, I will illustrate how information can be extracted from data by leveraging reduced representations, that is, by looking at the system under examination in terms of a wisely chosen subset of its constituents - be these atoms, spins, pixels, or else. Taking the moves from the theory of bottom-up coarse-graining in soft matter, it is possible to show that the level of resolution at which a system is described can be leveraged as a magnifying glass to investigate its properties, and that a precise notion of optimal resolution level can be given that is tightly connected with its key emergent features.

CPP 52: Focus Session: Ultrafast Processes in Organic Semiconductors and Perovskites III (joint session O/CPP)

Time: Friday 10:30–11:45 Location: MA 004

CPP 52.1 Fri 10:30 MA 004

Unveiling ultrafast vibronic dynamics in organic chromophores from first principles — •Michele Guerrini[1], Jannis Krumland[1,2], and Caterina Cocchi[1,2] — [1]Physics Department and Center for Nanoscale Dynamics(CeNaD), Carl von Ossietzky Universität Oldenburg, Germany — [2]Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Identifying and quantifying the interplay between electron and nuclear dynamics in the excited state of organic molecules is of paramount importance to unveil and interpret their complex photophysics upon ultrafast excitation. In this work, we investigate from first principles the ultrafast vibronic dynamics of p-coumaric acid chromophore [1]. We start off the simulations in excited states corresponding to bright or dark transitions. By monitoring the kinetic energy spectral density [2] and the population dynamics, we analyze the characteristics of the electron-nuclear motion and its evolution over a time window of 300 fs. We observe that anharmonic and non-adiabatic effects are particularly pronounced in excitations with charge-transfer character and lead to instabilities with the eventual distortion of the system. On the other hand, the dynamics initialized from bright excited states with delocalized character remains electronically and structurally stable, and the resulting nuclear motion is markedly harmonic.

[1] Theor. Chem. Acc. 142, 110 (2023)

[2] J. Phys. Chem. A, 125, 9619 (2021)

CPP 52.2 Fri 10:45 MA 004

Ultrafast Charge-Transfer in Spiro-Bridged Triphenylamine Derivatives Investigated by Broadband Transient Absorption Spectroscopy — •Danyellen Galindo[1], Angelina Jocic[2], Anna Weidlich Weidlich[3], Frank Rominger[2], Thomas Oeser[2], Jonathan Zerhoch[1], Felix Deschler[1], Andreas Drew[3], Milan Kivala[2], and Tiago Buckup[1] — [1]PCI, Universität Heidelberg, Heidelberg — [2]OCI, Universität Heidelberg, Heidelberg — [3]IWR, Universität Heidelberg, Heidelberg

Triphenylamine compounds (TPA) are studied in order to understand their photochemical processes such as charge transfer (CT). This investigation is motivated by their ability in stabilizing positive charges through a delocalize π-system, thereby facilitating hole transport. This work aimed to study the optical properties of Spiro-bridged Fluorene N-heterotriangulenes (FTN-H) and FTN-(CN)6. Both compounds, dissolved in dichloromethane (DCM), underwent transient absorption experiments with 300 nm excitation. Initial findings suggest that the solvent does not play a significant role in the CT process. The non-subsituted compound upon excitation simultaneously displayed S1 electronic band for the molecule core and fluorene side group, succeeded by a 2 ns inter-system crossing (ISC) transition, thus forming a triplet state T*1 that decays to S0 with time constant of 16 *s. FTN-(CN)6 exhibited overall comparable dynamics, but also displayed an ultrafast CT between S1 and T*1 states. Such CT, which can be observed in various donor-acceptor materials, hints at potential applications in solar energy conversion and storage systems.

CPP 52.3 Fri 11:00 MA 004

The effect of the acceptor strength on intramolecular charge separation in quadrupolar dye — •Somayeh Souri[1], Katrin WInte[1], Daniel Luenemann[1], Fulu Zheng[2], Mohamed Madjet[2], Teresa Kraus[3], Elena Mena-Osteritz[3], Peter Baeuerle[3], Sergei Tretiak[4], Antonietta De Sio[1], and Christoph Lienau[1] — [1]Oldenburg University, Germany — [2]Bremen University, Germany — [3]Ulm University, Germany — [4]Los Alamos National Laboratory, USA

Quadrupolar dyes, consisting of two terminal acceptors (A) linked to a central donor (D) are of high relevance for applications in nonlinear optics and photovoltaics. They recently demonstrated exceptional nonadiabatic quantum dynamics. In A-D-A thin films, we have uncovered the existence of intermolecular conical intersections, funneling energy into a lower-lying electronic state within less than 50 fs [1]. This raises the question how the strength of the acceptor group affects the quantum dynamics. Chemical intuition suggests that an increase in acceptor strength may accelerate charge transfer and increase its yield. We synthesize three A-D-A molecules with different acceptor strength and study them in polar solvents using ultrafast spectroscopy with 10fs time resolution. Even though we can distinguish between vibronic coupling-induced charge separation on a sub-100 fs scale and slower solvatochromism, we observe only weak effects of the acceptor group on the dynamics. The results suggest that vibronic coupling-induced excited state symmetry breaking plays a major role in quantum dynamics. [1] A. De Sio et al., Nature Nano 16, 63 (2021).

CPP 52.4 Fri 11:15 MA 004

Probing Site-Specific Photocatalytic Activity of Triazin-Based Graphitic Carbon Nitride via Time-Resolved and Resonant X-Ray Photoelectron Spectroscopy. — •Matz Nissen[1], Charlotte Ruhmlieb[1], Ivan Baev[1], Sebastian Denke[1], Lukas Wenthaus[3], Dmytro Kutnyakhov[3], Nils Wind[2,3], Federico Pressacco[3], Jens Buck[2], Steffen Palutke[4], Marion Kuhlmann[3], Günter Brenner[3], Kai Rossnagel[2,3], Alf Mews[1], and Michael Martins[1] — [1]Universität Hamburg, D — [2]Christian-Albrechts-Universität zu Kiel, D — [3]DESY, Hamburg, D — [4]European XFEL, Hamburg, D

Triazin-Based Graphitic Carbon Nitride (TGCN) has shown potential as a metal-free catalyst for photocatalytic water splitting, utilizing soley a visible light source and water. To gain further insight into the morphology of TGCN and the specific location where water binds during the catalytic reaction, we conducted resonant and time-resolved photoelectron spectroscopy of the carbon and nitrogen sites in a clean and a water environment. These experiments were done at beamline P04 of PETRAIII and beamline PG2 of FLASH respectively. Altering the sample environment shows differences in the resonant maps of the N K-edge. Additionally, time resolved measurements showed an excitation in the nitrogen spectra, specifically in the ring structure of the graphitic system. These results aim to help to improve the catalytic performance of the sample.

CPP 52.5 Fri 11:30 MA 004

Ultrafast dynamics in polymeric carbon nitride thin films probed by time-resolved extreme-ultraviolet photoemission spectroscopy — Nataliia Kuzkova[1,2], Igor Yu. Kiyan[1], Iain Wilkinson[1], and •Christoph Merschjann[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Advanced Research Center for Nanolithography, Science Park 106, 1098 XG Amsterdam, The Netherlands

Polymeric carbon nitrides (PCN) have been extensively studied for various possible applications, mainly in the field of photocatalysis, but also as potential organic semiconductors, luminescent materials, etc. Especially photocatalytic applications are affected by the apparently low charge-separation and transport efficiency of PCN. It is therefore of interest to investigate the early-time dynamics of photoexcited charge carriers, specifically at the surface of the photocatalyst. To this end, we applied femtosecond time-resolved pump-probe extreme-ultraviolet photoemission spectroscopy (TRPES) to differently synthesized PCN thin films. Excitation at 400 nm sequentially populates a pair of short-lived transient species, which subsequently produce two different long-lived excited states on a sub-picosecond time scale. These could be assigned to singlet-exciton and charge-transfer states with a high initial spatial correlation, respectively. The results also show the potential of TRPES as a tool for in-situ investigations of early-time dynamics in photocatalytic processes.

[1] Kuzkova et al., *Phys. Chem. Chem. Phys.*, **25**, 27094 (2023)

CPP 53: Responsive and Adaptive Systems II

Time: Friday 11:30–13:00 Location: H 0107

Invited Talk CPP 53.1 Fri 11:30 H 0107

A hierarchical fabrication strategy for multi-responsive actuators with structural reconfiguration-assisted self-healing ability — •Qing Chen — Laboratory for High Performance Ceramics, Empa, Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, 8600 Dübendorf, Switzerland

The prospects of endowing stimuli-responsive materials with various life-like behaviors are promoting the development of intelligent robotic and electronic systems. However, it is extremely challenging to incorporate stimuli-responsive actuating and healing ability into one single material system. Herein, we describe a general design strategy of a humidity-responsive thin film composed of conducting polymer composites through physically crosslinking and hydrogen bonding supramolecular network. Owing to the dynamic nature of hydrogen bonding at an elevated humidity, the thin film exhibits rapid actuating and efficient healing performance at the structural, mechanical and functional levels. Moreover, through a combined analytical approach, we proposed a structural model for the reconfiguration of the thin film at multi-length scales when being exposed to elevated humidity levels. Based on the humidity-responsive structural configurations, the film presents tunable mechanical, electrical and actuating properties, and demonstrate its great potential as intelligent soft robots such as artificial muscles.

CPP 53.2 Fri 12:00 H 0107

Dynamic Behavior of Poly(*N*-isopropylmethacrylamide) in Water/Methanol Mixtures — Chia-Hsin Ko[1], Patrick Wastian[1], Dirk Schanzenbach[2], André Laschewsky[2,3], Peter Müller-Buschbaum[1], and •Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Universität Potsdam, Institut für Chemie, Potsdam-Golm, Germany — [3]Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm

The thermoresponsive polymer poly(*N*-isopropylmethacrylamide) (PNIPMAM) features peculiar structural behavior [1]. Here, we investigate the dynamics of PNIPMAM in aqueous solution and in water/methanol mixtures in the one-phase region. Using dynamic light scattering, we observe two diffusive dynamic modes in a wide range of temperatures and polymer concentrations, which reflect local and large-scale dynamics. The scaling behavior of the dynamic correlation length of the fast mode deviates strongly from mean-field predictions, which may be related to the presence of the large-scale inhomogeneities, assigned to the enhanced hydrophobic effect. In water/methanol mixtures, the slow mode is strongly reduced, and the scaling exponent features non-monotonous behavior. Thus, the hydrophobic interactions result in complex behavior.

1. C.-H. Ko, C. M. Papadakis et al., *Macromolecules* **2020**, *53*, 6816.

CPP 53.3 Fri 12:15 H 0107

Local direction of opto-mechanical stress in azobenzene containing polymers during surface relief grating formation — •Sarah Loebner[1], Bharti Yadav[2], Nino Lomadze[1], Nina Tverdokhleb[2], Hendrik Donner[3], Marina Saphiannikova[2], and Svetlana Santer[1] — [1]Universität Potsdam, Potsdam, Germany — [2]Leibniz Institute of Polymer Research Dresden, Dresden, Germany — [3]CADFEM GmbH, Chemnitz, Germany

Here we unravel how the photo-induced deformation of azobenzene containing polymers relates to the local direction of opto-mechanical stresses generated during irradiation with interference patterns (IPs). We can substantiate the modeling approach in [1], that these deformations arise from the re-orientation of rigid backbone segments along the light polarization direction. In experiments we inscribe surface relief grating in pre-elongated photosensitive colloids of few micrometers using different IPs. The deformation of the colloidal particles is studied in-situ, whereby the local variation of the polymer topography is assigned to the local distribution of electrical field vector for all IPs. Orientation approach correctly predicts local variations of the main axis of light-induced stress in each interference pattern for both initially isotropic and highly oriented materials. With this work, we suggest that the orientation approach implements a self-sufficient and convincing mechanism to describe photo-induced deformation in azobenzene containing polymer films that does not require auxiliary assumptions.

[1] Yadav, B. et al., J. Phys. Chem. B 2019, 123, 3337-3347.

CPP 53.4 Fri 12:30 H 0107

Electroactive nanoporous silicon-polypyrrole hybrids in aqueous electrolytes: An in-situ high-resolution X-ray diffraction study — •Manuel Brinker[1,2] and Patrick Huber[1,2,3] — [1]Institut für Material- und Röntgenphysik, Technische Universität Hamburg, Denickestraße 15, 21073 Hamburg, Deutschland — [2]Deutsches Elektronen-Synchrotron DESY, Center for X-Ray and Nano Science CXNS, 22607 Hamburg, Deutschland — [3]Center for Hybrid Nanostructures CHyN, Universität Hamburg, 22607 Hamburg, Deutschland

A hybrid material of the electroactive polymer polypyrrole filled within the scaffold structure of the porous semiconductor porous silicon is exhibiting a reversible straining by control of an applied potential in an electrolyte solution. Anions from the electrolyte solution are inserted into or extracted from the polymer if it is polarized by an applied potential. This process is accompanied by an expansion or contraction of the polymer, which means a change of its geometrical dimensions. This process is directed by the confinement of the silicon nanopores. The swelling of the polymer impacts the mono-crystalline lattice in the porous silicon pore walls. Thus, it is possible to perform a highly resolved investigation of the reversible straining by means of an in-situ X-ray diffraction study that determines the lattice parameter inside the pore wall. [1]

[1] Manuel Brinker, Marc Thelen, Manfred May, Dagmar Rings, Tobias Krekeler, Pirmin Lakner, Thomas F. Keller, Florian Bertram, Norbert Huber, and Patrick Huber(2022). Physical Review Materials, 6(11), 116002.

CPP 53.5 Fri 12:45 H 0107

Self-assembled photonic pigments from bottlebrush block copolymers — •Ruiting Li[1], Zhen Wang[2], Richard Parker[2], and Silvia Vignolini[1,2] — [1]Department of Sustainable and Bioinspired Materials, Max-Planck Institute of Colloids and Interfaces, Potsdam, 14476, Germany — [2]Yusuf Hamied Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, UK

Bottlebrush block copolymers (BBCPs) have emerged as a versatile material for constructing photonic materials. In contrast to alternative photonic materials, BBCPs offers several distinct advantages, including: rapid assembly kinetics, ordering over macroscopic dimensions, and the capacity to accommodate substantial functionality.

In this talk we will introduce a robust strategy for the fabrication of hierarchical photonic pigments via the confined self-assembly of BBCPs within emulsified microdroplets. By optimising the BBCP composition and the emulsification conditions, we demonstrate that microparticles with a well-resolved concentric lamellar structure can be formed. The fundamental optical response (i.e. colour) is determined via the BBCP molecular weight, however we will show that by exploiting new macromonomers it is possible to produce ”photonic pigments” that are mechanochromic, unlocking potential application as ultrasensitive pressure sensors.

CPP 54: Closing Talk (joint session BP/CPP/DY)

Time: Friday 13:15–14:00 Location: H 0104

Invited Talk CPP 54.1 Fri 13:15 H 0104

Virus traps and other molecular machines of the future — •Hendrik Dietz — Technische Universität München, Garching b. München, Deutschland

Our interest is in learning how to build molecular devices and machines that can execute user-defined tasks. To this end, we investigate how to adapt the physical principles underlying the formation of natural macromolecular assemblies such as viruses or molecular motors for our purposes. Programmable molecular self-assembly with DNA origami is an attractive route toward implementing these principles to create synthetic molecular machinery. We combine computational design and cryo electron microscopy to learn how to construct synthetic molecular objects with increasing accuracy and increasing complexity.

For example, we have learned from viruses how to program DNA blocks to self-assemble into icosahedral shells with specific geometry and apertures, which led to an interesting application: the virus trap, which we hope to develop into a programmable antiviral drug to neutralize viruses. We have also learned how to design DNA origami so that genetic instructions included within them can be read by mammalian cells.

We also have recently learned how to control the movement of nanoscale assemblies. For example, we have built autonomous, power-generating rotary DNA motors driven by AC fields and also turbines that can be driven by ion flux across membranes. With these new machines, opportunities are created to accomplish user-defined, energy-consuming tasks in various contexts.