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

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Overview of Invited Talks and Sessions

(Lecture halls H34, H38, and H46; Poster P3 and P4)

Invited Talks

CPP 1.1	Mon	9:30–10:00	H34	**Impact of smallest loops and composition fluctuations on the structure of end-linked polymer model networks** — •Michael Lang, Reinhard Scholz, Toni Müller
CPP 5.1	Mon	11:30–12:00	H38	**Theoretical characterization of sulfur/carbon copolymer cathodes for next-generation batteries via *ab initio* spectroscopy simulations** — •Daniel Sebastiani, Pouya Partovi-Azar
CPP 8.1	Mon	15:00–15:30	H38	**The Nanoscale Photovoltaics Laboratory on a Tip** — •Stefan Weber
CPP 16.1	Tue	9:30–10:00	H34	**Multifunctional structural batteries** — •Göran Lindbergh
CPP 17.1	Tue	9:30–10:00	H38	**Continuum models for water's peculiar behavior on the nanoscale** — •Alexander Schlaich
CPP 18.1	Tue	9:30–10:00	H46	**Hybrid materials from colloidally stable nanocellulose and nanoparticles - scattering techniques are needed for characterization** — •Eva Malmström, Åsa Jerlhagen, Benedikt Sochor, Korneliya Gordeyeva, Stephan Roth
CPP 20.1	Tue	11:30–12:00	H38	**Tailored polymer thin films enabled by initiated chemical vapor deposition (iCVD): From fundamentals to functional applications** — •Stefan Schröder
CPP 23.1	Wed	9:30–10:00	H34	**Advanced combined rheometer setups to in-situ correlate molecular dynamics and molecular structure formation with mechanical properties** — •Manfred Wilhelm
CPP 26.1	Wed	11:30–12:00	H34	**Polyelectrolytes in the confined space of mesopores for transport regulation** — •Annette Andrieu-Brunsen
CPP 30.1	Wed	16:15–16:45	H34	**Challenges and Opportunities in Bringing Machine Learning to a Synchrotron** — •Alexander Hexemer, Tanny Chavez, Wiebke Köpp, Dylan McReynolds, Stephan Roth, Tim Snow, Sharif Ahmed
CPP 31.1	Wed	16:15–16:45	H38	**Moving with minimum effort – Optimal work protocols for systems with memory** — •Sarah Loos, Samuel Monter, Felix Ginot, Clemens Bechinger
CPP 34.1	Thu	15:00–15:30	H34	**Understanding Nanocellulose-Water Interactions to Engineer Advanced Functional Materials** — •Valentina Guccini
CPP 37.1	Thu	16:15–16:45	H34	**Modelling Hygroexpansion of Compression and Opposite Wood of Conifer Branches: Bridging the Gap between Molecular and Cell Wall Level** — Marie Hartwig-Nair, Sara Florisson, Kristofer Gamstedt, •Malin Wohlert
CPP 38.1	Thu	16:15–16:45	H38	**Adsorption and Interaction of Amino Acids on Titanium Oxide Photocatalyst** — Miguel Blanco-Garcia, Mona Kohantorabi, Benedikt Socher, Ulrike Protzer, Stephan V. Roth, Cristiana Di Valentin, Andreas Stierle, •Heshmat Noei
CPP 41.1	Fri	9:30–10:00	H38	**Simulations of reaction equilibria in macromolecular systems** — •Peter Košovan

Invited Talks of the joint Symposium Physics of Embryonic Development Across Scales: From

DNA to Organisms (SYED)

See SYED for the full program of the symposium.

SYED 1.1	Mon	9:30–10:00	H1	**Emergent crystalline order in a developing epithelium** — Kartik Chhajed, Natalie Dye, Marko Popović, •Frank Jülicher
SYED 1.2	Mon	10:00–10:30	H1	**A tissue rigidity phase transition shapes morphogen gradients** — Camilla Autorino, Diana Khoromskaia, Bernat Corominas-Murtra, Zena Hadjivasiliou, •Nicoletta Petridou
SYED 1.3	Mon	10:30–11:00	H1	**Building quantitative dynamical landscapes of developmental cell fate decisions** — •David Rand
SYED 1.4	Mon	11:15–11:45	H1	**Control of lumen geometry and topology by the interplay between pressure and cell proliferation rate** — •Anne Grapin-Botton, Byung Ho Lee, Masaki Sano, Daniel Riveline, Kana Fuji, Tetsuya Hiraiwa
SYED 1.5	Mon	11:45–12:15	H1	**Chromosomes as active communication and memory machines** — •Leonid A. Mirny

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium Pushing the Boundaries of Fair Data Practices for Condensed Matter Insights: From Workflows to Machine Learning (SYFD)

See SYFD for the full program of the symposium.

SYFD 1.1	Wed	9:30–10:00	H1	**Pushing the Boundaries of Fair Data Practices for Condensed Matter Insight** — •Astrid Schneidwind
SYFD 1.2	Wed	10:00–10:30	H1	**Establishing Workflows of Experimental Solar Cell Data into NOMAD** — Edgar Nandayapa, Paolo Graniero, Jose Marquez, Michael Götte, •Eva Unger
SYFD 1.3	Wed	10:30–11:00	H1	**Building up the EOSC Federation** — •Ute Gunsenheimer
SYFD 1.4	Wed	11:15–11:45	H1	**Data-Driven Materials Science for Energy-Sustainable Applications** — •Jacqueline Cole
SYFD 1.5	Wed	11:45–12:15	H1	**Machine Learning and FAIR Data in X-ray Surface Science** — •Stefan Kowarik

Invited Talks of the joint Symposium AI in (Bio-)Physics (SYAI)

See SYAI for the full program of the symposium.

SYAI 1.1	Thu	9:30–10:00	H1	**Predicting interaction partners and generating new protein sequences using protein language models** — •Anne-Florence Bitbol
SYAI 1.2	Thu	10:00–10:30	H1	**Realizing Schrödinger's dream with AI-enabled molecular dynamics** — •Alexandre Tkatchenko
SYAI 1.3	Thu	10:30–11:00	H1	**Emergent behavior of artificial intelligence** — •Steffen Rulands
SYAI 1.4	Thu	11:15–11:45	H1	**AI in medical research - navigating complexity with AI** — •Daniel Truhn
SYAI 1.5	Thu	11:45–12:15	H1	**Computational Modelling of Morphogenesis** — •Dagmar Iber

Sessions

CPP 1.1–1.6	Mon	9:30–11:15	H34	**Gels, Polymers Networks and Elastomers I**
CPP 2.1–2.11	Mon	9:30–12:45	H37	**Active Matter I (joint session DY/BP/CPP)**
CPP 3.1–3.7	Mon	9:30–11:15	H38	**Organic Electronics and Photovoltaics I**
CPP 4.1–4.6	Mon	11:30–13:00	H34	**Crystallization, Nucleation and Self-Assembly I**
CPP 5.1–5.5	Mon	11:30–13:00	H38	**Composites and Functional Polymer Hybrids**
CPP 6.1–6.4	Mon	15:00–16:00	H34	**Gels, Polymers Networks and Elastomers II**
CPP 7.1–7.7	Mon	15:00–17:00	H37	**Active Matter II (joint session BP/CPP/DY)**
CPP 8.1–8.3	Mon	15:00–16:00	H38	**Hybrid and Perovskite Photovoltaics I**
CPP 9.1–9.6	Mon	15:00–16:45	H46	**Biomaterials and Biopolymers (joint session BP/CPP)**
CPP 10.1–10.4	Mon	16:15–17:15	H34	**Wetting, Fluidics and Liquids at Interfaces and Surfaces I (joint session CPP/DY)**
CPP 11.1–11.3	Mon	16:15–17:00	H38	**Hybrid and Perovskite Photovoltaics II**
CPP 12.1–12.4	Mon	17:00–18:00	H46	**Biomaterials, Biopolymers and Bioinspired Functional Materials I (joint session CPP/BP)**
CPP 13.1–13.5	Mon	17:15–18:30	H38	**Molecular Electronics and Excited State Properties I**
CPP 14.1–14.4	Mon	17:30–18:30	H34	**Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)**
CPP 15.1–15.74	Mon	19:00–21:00	P4	**Poster Session I**
CPP 16.1–16.6	Tue	9:30–11:15	H34	**Energy Storage and Batteries I**
CPP 17.1–17.6	Tue	9:30–11:15	H38	**Modeling and Simulation of Soft Matter I**
CPP 18.1–18.6	Tue	9:30–11:15	H46	**Biomaterials, Biopolymers and Bioinspired Functional Materials II (joint session CPP/BP)**
CPP 19.1–19.11	Tue	9:30–13:00	H47	**Active Matter III (joint session DY/BP/CPP)**
CPP 20.1–20.5	Tue	11:30–13:00	H38	**Interfaces and Thin Films I**
CPP 21.1–21.6	Tue	14:00–15:30	H34	**Modeling and Simulation of Soft Matter II**
CPP 22.1–22.5	Tue	14:00–15:15	H38	**Organic Electronics and Photovoltaics II**
CPP 23.1–23.6	Wed	9:30–11:15	H34	**Polymer and Molecular Dynamics, Friction and Rheology**
CPP 24.1–24.7	Wed	9:30–11:15	H38	**Hybrid and Perovskite Photovoltaics III**
CPP 25.1–25.20	Wed	10:00–12:00	P3	**Poster: Active Matter, Soft Matter, Fluids (joint session DY/CPP)**
CPP 26.1–26.5	Wed	11:30–13:00	H34	**Nanostructures, Nanostructuring and Nanosized Soft Matter I**
CPP 27.1–27.6	Wed	11:30–13:00	H38	**Molecular Electronics and Excited State Properties II**
CPP 28.1–28.4	Wed	15:00–16:00	H34	**Modeling and Simulation of Soft Matter III**
CPP 29.1–29.4	Wed	15:00–16:00	H38	**Organic Electronics and Photovoltaics III**
CPP 30.1–30.8	Wed	16:15–18:30	H34	**Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods I**
CPP 31.1–31.6	Wed	16:15–18:00	H38	**Responsive and Adaptive Polymers**
CPP 32.1–32.45	Thu	9:30–12:00	P3	**Poster Session II**
CPP 33.1–33.5	Thu	11:45–13:00	H34	**Modeling and Simulation of Soft Matter IV**
CPP 34.1–34.3	Thu	15:00–16:00	H34	**Focus Session: Interactions Between Water and Cellulose I**
CPP 35.1–35.9	Thu	15:00–17:45	H37	**Microswimmers and Microfluidics (joint session DY/BP/CPP)**
CPP 36.1–36.4	Thu	15:00–16:00	H38	**Organic Electronics and Photovoltaics IV**
CPP 37.1–37.3	Thu	16:15–17:15	H34	**Focus Session: Interactions Between Water and Cellulose II**
CPP 38.1–38.5	Thu	16:15–17:45	H38	**Interfaces and Thin Films II**
CPP 39	Thu	18:00–19:00	H38	**Members' Assembly**
CPP 40.1–40.7	Fri	9:30–11:15	H34	**Energy Storage and Batteries II**
CPP 41.1–41.6	Fri	9:30–11:15	H38	**Charged Soft Matter, Polyelectrolytes and Ionic Liquids I**
CPP 42.1–42.12	Fri	9:30–13:00	H44	**Active Matter IV (joint session BP/CPP/DY)**
CPP 43.1–43.11	Fri	9:30–12:45	H47	**Droplets, Wetting, Complex Fluids, and Soft Matter (joint session DY/CPP)**
CPP 44.1–44.4	Fri	11:30–12:30	H34	**2D Materials**
CPP 45.1–45.5	Fri	11:30–12:45	H38	**Charged Soft Matter, Polyelectrolytes and Ionic Liquids II**
CPP 46.1–46.1	Fri	13:15–14:00	H2	**Closing Talk (joint session BP/CPP/DY)**

Members' Assembly of the Chemical and Polymer Physics Division

Thursday 18:00–19:00 H38

CPP 1: Gels, Polymers Networks and Elastomers I

Time: Monday 9:30–11:15 Location: H34

Invited Talk CPP 1.1 Mon 9:30 H34

Impact of smallest loops and composition fluctuations on the structure of end-linked polymer model networks — •Michael Lang, Reinhard Scholz, and Toni Müller — Leibniz-Institut für Polymerforschung, Dresden, Germany

A self-consistent scheme of differential equations is developed for predicting the frequency of the two smallest loop defects within polymer model networks. Without any adjustable parameter, we obtain excellent agreement with Monte Carlo simulations that sample loop formation only up to the given maximum loop size. The formation of loops of second generation leads to correlations between connected junctions that cannot be treated exactly by considering statistical arguments alone, which is in contrast to reversible networks where equilibrium statistics are sufficient. These correlations and the statistics of the junctions are provided by our model. Comparison with more realistic simulation data in three dimensions indicates that composition fluctuations of cross-links and chains clearly impact network formation. The differences between the statistics of the network junctions and our mean field predictions provide insight into the size of the domains with a predominance of chains or junctions and thus, regarding the quality of the mixture. Our results are highly relevant for an accurate modeling of network structure, improved estimates of the elastic properties of polymer networks, and for advanced analysis techniques of the network structure like network disassembly spectrometry or multiple quantum nuclear magnetic resonance.

CPP 1.2 Mon 10:00 H34

Hybrid PNIPAM Films for Green Hydrogen Production — •Morgan P. Le Dû[1], David P. Kosbahn[1], Thomas Baier[1], Qi Zhong[2], Apostolos Vagias[3], Robert Cubitt[3], Narendra Chaulagain[4], Karthik Shankar[4], Hagen Übele[5], Katharina Krischer[5], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Zhejiang Sci-Tech University, Hangzhou, China — [3]Institut Laue-Langevin (ILL), Grenoble, France — [4]University of Alberta, Department of Electrical and Computer Engineering, Edmonton, Canada — [5]TUM School of Natural Sciences, Nonequilibrium Chemical Physics, 85748 Garching, Germany

Platinum (Pt) doped carbon nitride (CN) is a promising photocatalyst under visible light for green hydrogen (H2) production. We develop this system in a thin polymer film to make it industrially scalable. The poly(N-isopropylacrylamide) (PNIPAM) hydrogel is used as a host matrix and water storage medium to facilitate homogeneous dispersion of the catalytic centers. The hybrid film's vertical distribution and inner microstructure are studied under in situ conditions with time-of-flight neutron reflectometry (ToF NR) and grazing incidence small angle neutron scattering (GISANS). The resulting H2 produced is measured by gas chromatography.

CPP 1.3 Mon 10:15 H34

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

We investigate the properties of polyelectrolyte hydrogels with various network heterogeneities, particularly their swelling capacity, elastic modulus and salt partitioning. We benchmark the scaling predictions for elastic modulus and equilibrium swelling ratio of the hydrogels under various salinity conditions, verifying the theoretically predicted behavior. Decoupling the elastic modulus from the swelling behavior is beneficial for applications such as super absorbers. Here, for example, now wants to increase the swelling ratio while maintaining a reasonable mechanical strength. We therefore explore mechanical and structural properties of the hydrogels with varying topologies, namely gels with dangling ends, gels with floating chains, and bottle-brush gels in counterpart to a reference regular gel. We observe that incorporating dangling ends changed swelling ratio and bulk modulus inline with the scaling predictions, whereas bottle-brush and floating-chain gels deviate from the predictions. Specifically, floating chains resulted in higher moduli and higher swelling ratio, while bottle-brush gels resulted in lower moduli and lower swelling ratios than the regular counterpart, each maintaining the same swelling ratio and modulus. The new swelling-mechanical relations allow us to treat them in a decoupled manner via the topology variation, which turns out to be of paramount relevance in the optimization and on-demand design of hydrogels.

CPP 1.4 Mon 10:30 H34

Aqueous foams stabilized by PNIPAM microgels: A multiscale investigation — •Joanne Zimmer, Luca Mirau, Gaëtan Barth, and Regine von Klitzing — Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 8, D-64289 Darmstadt

Foams possess several structural motifs on different length scales with the smallest building blocks being the foam films or even the liquid/air interface. In this work, PNIPAM microgels (MG) are used as foam stabilizers as they are highly interfacial active and temperature responsive. In addition, the MG stiffness and by this their interfacial activity can be tuned by variation of the crosslinker content. We present a multi-scale approach towards understanding how the MG properties are related to the macroscopic foam and foam film stability. Spatially resolved disjoining pressure isotherms are measured with a Thin Film Pressure Balance (TFPB). The isotherms provide information about the film thickness, surface mobility and film stability. These properties are correlated with macroscopic foam characteristics such as foamability, stability and drainage dynamics. Indeed, the results are in good agreement on all length scales: A lower crosslinker content supports foam formation due to a faster surface coverage and results in an increased foam stability, as a more rigid surface layer is formed. Increasing the amount of crosslinker in the MG induces a transition from Poiseuille flow to plug flow in the foam during drainage which coincides with an increasing mobility of the surface of a single foam film measured in a TFPB.

CPP 1.5 Mon 10:45 H34

Phase separation in elastic polymer networks — •Takahiro Yokoyama[1,2], Yicheng Qiang[3], Chengjie Luo[3], Oliver Paulin[3], David Zwicker[3], and Arash Nikoubashman[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany

Phase separation in polymer networks, from synthetic gels to biopolymer networks, significantly influences their structural and mechanical properties. While previous studies suggest that network mechanics regulate phase separation of the network itself and the embedded (complex) liquid, the fundamental principles governing this interaction remain poorly understood. To address this knowledge gap, we used molecular dynamics (MD) simulations to explore the phase behavior of elastic polymer networks. We systematically changed the quality of the (implicit) solvent, polymer chain length, and polymer flexibility. Our simulations identified two distinct phase separation behaviors depending on the polymer flexibility: macrophase separation into a polymer-rich and polymer-poor region for flexible polymer chains, and microphase separation with finite-sized pores for networks formed by semi-flexible chains. For the latter systems, we found that the pore size decreased with increasing chain stiffness. Furthermore, the network elasticity increased with decreasing pore size, following a power law as recently proposed by field theory. This study highlights the importance of polymer stiffness in shaping the size and distribution of (biomolecular) droplets within elastic networks.

CPP 1.6 Mon 11:00 H34

Nanoscopic measurements of the water content in microgels using fluorescence lifetime imaging — •Dominik Wöll[1], Alexandre Fürstenberg[2], Jörg Enderlein[3], Oleksii Nevskyi[3], Sankar Jana[1], Hannah Höche[1], and Leon Trottenberg[1] — [1]RWTH Aachen University, Institute of Physical Chemistry, Aachen, Germany — [2]University of Geneva, Department of Physical Chemistry and Department of Inorganic and Analytical Chemistry, Genf, Switzerland — [3]Georg August University, 3rd Institute of Physics - Biophysics, Göttingen, Germany

The role of water molecules in the structure, function, and dynamics of (bio-)materials is significant, and thus, an estimation of the number of water molecules within different compartments is crucial. It has been demonstrated that the fluorescence of red emissive dyes is quenched in the presence of H_2O, with the excited energy transferred to surrounding H_2O molecules. Fluorescence lifetime imaging (FLIM) can thus be used to quantify the number of water molecules in proximity to the probing dye Atto 655, which was covalently embedded into microgels in the present study. Microgels represent an intriguing class of nanoparticles with considerable potential for applications in drug delivery and medicinal chemistry. We recorded FLIM images at varying H_2O:D_2O ratios, in both the swollen and collapsed states of the microgels at 22 °C and 40 °C, respectively. Stern-Volmer analysis enabled the calculation of the number of water molecules in the immediate vicinity of the dye molecule within the microgels at varying temperatures.

CPP 2: Active Matter I (joint session DY/BP/CPP)

Time: Monday 9:30–12:45 Location: H37

CPP 2.1 Mon 9:30 H37

Odd dynamics and pattern formation in mixtures of magnetic spinners and passive colloids — •Dennis Schorn[1], Stijn van der Ham[2], Hanumantha Rao Vutukuri[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, 64289 Darmstadt, Germany — [2]MESA+ Institute, University of Twente, 7500 AE Enschede, The Netherlands

Starfish embryos aggregate into chiral crystals exhibiting odd elasticity (Tan *et al.* Nature **607**, 287 (2022)). Similar structures have been recently observed in externally driven magnetic colloids. In this talk, I present experiments and simulations of binary mixtures of magnetic spinners and passive colloids. We develop a model to predict the phase diagram of the system, which comprises four distinct phases that can be systematically reproduced in experiments. In particular, our simulations and experiments show a phase where the passive particles form a gel-like network featuring significant holes filled with self-organized rotating chiral clusters made of spinners. This phase can be reversed by changing the system's composition and magnetic field strength, featuring a system spanning spinner phase with embedded counter-rotating chiral clusters made of passive colloids. Our system may open the route towards a new type of viscoelastic active chiral matter involving nonreciprocal interactions between both species.

CPP 2.2 Mon 9:45 H37

Symmetry breaking in active non-reciprocal systems — •Kim L. Kreienkamp and Sabine H. L. Klapp — TU Berlin, Germany

Non-reciprocity significantly impacts the dynamical behavior in mixtures. One of its particularly striking consequences is the spontaneous emergence of time-dependent phases that break parity-time symmetry [1-3]. Here, we study a paradigmatic model of a non-reciprocal polar active mixture with completely symmetric repulsion [4,5]. Using a combination of field theory and particle-based simulations, we identify two qualitatively distinct regimes of non-reciprocity-induced dynamics. In the regime of weak intra-species alignment, non-reciprocity leads to asymmetric clustering in which only one of the two species forms clusters. Notably, the asymmetric density dynamics is driven alone by non-reciprocal orientational couplings [4,5]. In contrast, in the strongly coupled regime, the corresponding field theory exhibits exceptional points that have been associated with the emergence of chiral phases where the polarization direction rotates over time [2]. Our simulations confirm that spontaneous chirality arises at the particle level. In particular, we observe chimera-like states with coexisting locally synchronized and disordered regions. At the coupling strengths associated with exceptional points, the spontaneous chirality peaks.

[1] Z. You et al., PNAS 117, 19767 (2020).
[2] M. Fruchart et al., Nature 592, 363 (2021).
[3] K. L. Kreienkamp and S. H. L. Klapp, NJP 24, 123009 (2022).
[4] K. L. Kreienkamp and S. H. L. Klapp, to appear in PRE (2024).
[5] K. L. Kreienkamp and S. H. L. Klapp, to appear in PRL (2024).

CPP 2.3 Mon 10:00 H37

Emergent phases in a discrete flocking model with non-reciprocal interaction — •Swarnajit Chatterjee, Matthieu Mangeat, and Heiko Rieger — Center for Biophysics & Department for Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

Non-reciprocal interactions arise in systems that seemingly violate Newton's third law "actio=reactio". They are ubiquitous in active and living systems that break detailed balance at the microscale, from social forces to antagonistic interspecies interactions in bacteria. Non-reciprocity affects non-equilibrium phase transitions and pattern formation in active matter and represents a rapidly growing research focus in the field. In this work, we have undertaken a comprehensive study of the non-reciprocal two-species active Ising model (NRTSAIM), a non-reciprocal discrete-symmetry flocking model. Our study uncovers a distinctive *run-and-chase* dynamical state that emerges under significant non-reciprocal frustration. In this state, A-particles chase B-particles to align with them, while B-particles avoid A-particles, resulting in B-particle accumulation at the opposite end of the advancing A-band. This run-and-chase state represents a non-reciprocal discrete-symmetry analog of the chiral phase seen in the non-reciprocal Vicsek model. Additionally, we find that self-propulsion destroys the oscillatory state obtained for the non-motile case, and all the NRTSAIM steady-states are metastable due to spontaneous droplet excitation and exhibit motility-induced interface pinning. A hydrodynamic theory supports our simulations and confirms the reported phase diagrams.

CPP 2.4 Mon 10:15 H37

Emergent phases in a discrete flocking model with reciprocal interaction — •Matthieu Mangeat[1], Swarnajit Chatterjee[1], Jae Dong Noh[2], and Heiko Rieger[1] — [1]Saarland University, Saarbrücken, Germany — [2]University of Seoul, Seoul, Korea

We have undertaken a comprehensive study of the two-species active Ising model (TSAIM), a discrete-symmetry counterpart of the continuous-symmetry two-species Vicsek model, motivated by recent interest in the impact of complex and heterogeneous interactions on active matter systems. In the TSAIM, two species of self-propelled particles undergo biased diffusion in two dimensions, interacting via local intraspecies alignment and reciprocal interspecies anti-alignment, along with the possibility of species interconversion. We observe a liquid-gas phase transition, exhibiting macrophase-separated bands, and the emergence of a high-density parallel flocking state, a feature not seen in previous flocking models. With species interconversion (species-flip dynamics), the TSAIM corresponds to an active extension of the Ashkin-Teller model and exhibits a broader range of steady-state phases, including microphase-separated bands that further enrich the coexistence region. We also find that the system is metastable due to droplet excitation and exhibits spontaneous motility-induced interface pinning, preventing the system from reaching long-range order at sufficiently low noise. A hydrodynamic theory complements our computer simulations of the microscopic model and confirms the reported phase diagrams.

CPP 2.5 Mon 10:30 H37

Emergent collective behavior from cohesion and alignment — •Jeanine Shea and Holger Stark — Technische Universität Berlin, Institut für Theoretische Physik, Hardenbergstr. 36, 10623 Berlin, Germany.

Collective behavior is all around us, from flocks of birds to schools of fish. These systems are immensely complex. To explore their basic characteristics, we introduce a minimal model for cohesive and aligning self-propelled particles in which group cohesion is established through additive, non-reciprocal torques [1]. These torques cause constituents to effectively turn towards one another, while an additional alignment torque competes in the same spatial range. By changing the strength and range of these torque interactions, we uncover six states which we distinguish via their static and dynamic properties. These states range from disperse particles to closely packed worm-like formations. A number of the states generated by this model exhibit collective dynamics which are reminiscent of those seen in nature.

[1] Knežević, M., Welker, T. and Stark, H. Collective motion of active particles exhibiting non-reciprocal orientational interactions. Sci Rep 12, 19437 (2022).

Invited Talk CPP 2.6 Mon 10:45 H37

Collective behavior of photoactive macroscopic particles —

•Iker Zuriguel — University of Navarra, Pamplona, Spain

Active matter refers to systems of interacting, self-propelled agents that convert energy into mechanical motion, representing a nice example of out-of-equilibrium systems. In this work, a novel type of active particles is introduced. These are active granular (i.e. they interact solely through physical contacts) and photoactive, meaning that they self-propel using energy from light. Therefore, by means of a programmable LED panel, we are able to change the illumination pattern and, consequently, the particle activity in space and time, allowing a precise exploration of a variety of scenarios related to collective behavior. This possibility has been exploited in microscopic systems but is genuinely new in macroscopic ones.

First, we will present the clustering behavior of these agents under homogeneous illumination. By varying the illumination intensities and changing the population size, we observed a power-law-like distribution for both the cluster sizes and durations. We identified a transition from unstable to stable clusters, as indicated by the divergence of average cluster durations. Higher particle activities and smaller populations led to the creation of small unstable clusters, while lower particle activities and larger populations result in big, stable clusters that persist over time. This transition is explained with the help of a simple model capturing the most important processes involved in cluster dynamics. In the last part of the talk, the collective behavior under inhomogeneous illumination patterns will be introduced.

15 min. break

CPP 2.7 Mon 11:30 H37

Swarming model with minority interaction exhibits temporal and spatial scale-free correlations — •Simon Syga[1], Chandraniva Guha Ray[2,3,4], Josué Manik Nava Sedeño[5], Fernando Peruani[6,7], and Andreas Deutsch[1] — [1]Technische Universität Dresden — [2]Max Planck Institute for the Physics of Complex Systems — [3]Max Planck Institute of Molecular Cell Biology and Genetics — [4]Center for Systems Biology Dresden — [5]Universidad Nacional Autónoma de México — [6]Université Côte d'Azur, Nice — [7]CY Cergy Paris Université

Collective motion is a widespread phenomenon in social organisms, from bird flocks and fish schools to human crowds and cell groups. Swarms of birds and fish are particularly fascinating for their coordinated behavior and rapid escape maneuvers during predator attacks. Critical motion is hypothesized as an optimal trade-off between cohesive group behavior and responsiveness to well-informed individuals. However, traditional models only show criticality at the phase transition between ordered and unordered motion. Here, we extend the Vicsek model with a minority interaction, where individuals primarily follow neighbors but can switch to follow a defector moving against a well-aligned group. This triggers cascades of defections, leading to rich dynamics, including large-scale fluctuations, scale-free velocity distributions, and a scale-free return time distribution of the order parameter. Our model underscores the biological importance of minority interactions in swarming and their role in critical behavior.

CPP 2.8 Mon 11:45 H37

'Predator-prey' driven swarmalator systems — •Ginger E. Lau, Mario U. Gaimann, and Miriam Klopotek — Stuttgart Center for Simulation Science (SimTech), Cluster of Excellence EXC 2075, University of Stuttgart, Germany

Swarmalators are an active matter system of oscillators which exhibit swarming and collective motion in physical space, as well as synchronization behavior in an additional phase variable space, originally introduced by O'Keeffe *et al.* (*Nat. Commun.* 8(1), 1504, 2017). Such systems with bidirectional couplings in space and phase can be observed in nature, such as in the chorusing behavior of Japanese tree frogs characterized by Aihara *et al.* (*Sci. Rep.* 4(1), 3891, 2014). The interplay between attraction, repulsion, and phase synchronization provides several distinct regimes of self-organizational behavior. Akin to biological swarm systems responding to predator interactions, swarmalators can respond collectively to external perturbations by a repulsive driver. In previous work, driving was realized with a mobile 'pacemaker' by Xu *et al.* (*Chaos* 34(11), 113103, 2024). The present study introduces a new 'predator-prey' driven swarmalator model showing rich adaptive behavior. This could have a wide variety of potential future applications, from biological physics to swarm robotics to nature-inspired learning algorithms and methods of inference.

CPP 2.9 Mon 12:00 H37

Inertial active matter governed by Coulomb friction — •Alexander Antonov[1], Lorenzo Caprini[2], and Hartmut Löwen[1] — [1]Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany — [2]University of Rome La Sapenzia, Rome, Italy

Coulomb, or dry friction, is a common phenomenon that can be encountered in various systems, such as granular matter or Brownian motors. The Coulomb friction force resists the motion and, unlike the friction in wet systems, is almost independent of the relative velocity. We show that this characteristic feature of Coulomb friction leads to emergence of dynamical states when subjected to active, or self-propelled motion [1]. At low activity levels, the dynamics resembles Brownian motion, while at greater activity, a dynamic Stop & Go regime emerges, marked by continuous switching between diffusion and accelerated motion. At even higher activity levels, a super-mobile regime arises, characterized by fully accelerated motion and an anomalous scaling of the diffusion coefficient with activity. Near the transition between the Stop & Go and super-mobile regimes, we reveal a novel activity-induced phase separation in collective behavior [2]. Our theoretical findings have been also demonstrated in experiments, where vibrobots on a horizontal surface are activated by vertical oscillations generated using an electromagnetic shaker.

[1] A.P. Antonov, L. Caprini, A. Ldov, C. Scholz, and H. Löwen, Phys. Rev. Lett. 133, 198301 (2024)

[2] A.P. Antonov et al., in preparation.

CPP 2.10 Mon 12:15 H37

Active nematic turbulence with substrate friction — •Peter A. E. Hampshire[1,2] and Ricard Alert[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Center for Systems Biology Dresden, Dresden, Germany — [3]Cluster of Excellence Physics of Life, Dresden, Germany

Active nematics with high activity exhibit turbulent-like flows, characterized by vortices, spatio-temporal chaos and power laws in the energy spectra [1-3]. Continuum models have been successfully used to predict the scaling of the energy spectra with the wavevector. Most theoretical work has focused on free-standing, active nematic films. However, in several experimental realisations, such as bacterial colonies and epithelial monolayers, the active nematic is in contact with a solid substrate. We generalised a 2D, incompressible active nematic model to include substrate friction, and studied its impact on the transition to turbulence and the energy spectra of the turbulent-like flows. We find a variety of dynamic states including flow in lanes, stable vortices and both isotropic and anisotropic turbulence. At high activity and moderate friction, we found a power-law scaling in the kinetic energy spectrum $E(q) \sim q^3$, where q is the wavevector, at low wavevectors. The exponent of 3 can be justified with a power-counting argument. Overall, we have developed a model for active nematic turbulence on a substrate that can be compared to biological systems. [1] L. Giomi, *Phys. Rev. X* **5**, 031003 (2015). [2] R. Alert, J.-F. Joanny, J. Casademunt, *Nat. Phys.* **16**, 682-688 (2020). [3] B. Martínez-Prat*, R. Alert*, et al., *Phys. Rev. X* **11**, 031065 (2021).

CPP 2.11 Mon 12:30 H37

Self-sustained patchy turbulence in shear-thinning active fluids — •Henning Reinken and Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg

Bacterial suspensions and other active fluids are known to develop highly dynamical vortex states, denoted as active or mesoscale turbulence. We reveal the pronounced effect of non-Newtonian rheology of the carrier fluid on these turbulent states, concentrating on shear thinning. As a consequence, a self-sustained heterogeneous state of coexisting turbulent and quiescent areas develops, which results in anomalous velocity statistics. The heterogeneous state emerges in a hysteretic transition under varying activity. We provide an extensive numerical analysis and find indirect evidence for a directed percolation transition. Our results are important, for instance, when addressing active objects in biological media with complex rheological properties.

CPP 3: Organic Electronics and Photovoltaics I

Time: Monday 9:30–11:15 Location: H38

CPP 3.1 Mon 9:30 H38

Demonstration of flexible organic solar cells in space — •Lukas V. Spanier[1], Lennart K. Reb[2], Michael Böhmer[3], Zerui Li[1], Christoph Dreissigacker[4], Thomas Voigtmann[4], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]TUM School of Natural Sciences, Zentrales Technologielabor, Garching, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [4]DLR Institut für Materialphysik im Weltraum, Köln, Germany

The deployment of flexible organic solar cells (OSCs) in space presents a transformative opportunity for exceptionally lightweight power generation on satellites and deep space research probes, promising record-breaking gravimetric power densities. In this study, we report the successfull launch, operation and recovery of flexible PEN-based OSCs on a suborbital rocket launch, assessing their performance in the harsh conditions of space. Flexible OSC modules were integrated into the payload and exposed to vacuum, microgravity, and cosmic radiation during the flight. Post-flight analysis of the recovered cells further confirmed the cells' operational viability. The experiment demonstrates the potential of OSCs for reducing launch mass and enabling novel satellite architectures, paving the way for their adoption in future space missions.

CPP 3.2 Mon 9:45 H38

Evaluate the energy losses in non-fullerene based organic photovoltaic — •Maryam Alqurashi[1], Shahidul Alam[2], Jose Jurado[1], Julien Gorenflot[1], and Frederic Laquai[1,2] — [1]Division of Physical Sciences and Engineering, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia — [2]Physical Chemistry and Spectroscopy of Energy Materials, Department of Chemistry, Ludwig Maximilian University of Munich, D-81377 Munich, Germany

Organic photovoltaics that use non-fullerene acceptors are gaining popularity because they can potentially increase power conversion efficiency. However, they suffer from significantly higher total energy losses than inorganic photovoltaics, primarily due to non-radiative recombination, a process in which electron-hole pairs recombine without generating current. Electroluminescence spectroscopy helps evaluate charge transfer state energy, which is crucial in charge recombination. This study focused on three systems: PM6:Y6, PM6:IT-4F, and PM6:ITIC. The PM6:Y6-based device showed higher radiative recombination, while the PM6:IT-4F system exhibited the highest order of non-radiative recombination. The total open circuit voltage losses were 0.64 eV, 0.67 eV, and 0.56 eV for PM6:Y6, PM6:IT-4F, and PM6:ITIC, respectively. Despite PM6:Y6 achieving a higher power conversion efficiency, its open circuit voltage losses were comparable to that of the other two systems.

CPP 3.3 Mon 10:00 H38

Towards printing of organic solar cells out of green solvents — •Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Despite big achievements in terms of power conversion efficiencies in the last years, with champion efficiencies above the 20% limit, it remains an unresolved challenge to fabricate large-area organic solar cells without sacrificing efficiencies. Large-area deposition of the conjugated polymer donor and small molecule acceptor blends via printing is key in the device upscaling. Another issue calling the attention is the fabrication of environmentally friendly organic solar cells. To become environmental-friendly, the used solvents are a key factor. Today, still the most used solvents are harmful and can cause environmental pollution during the device fabrication process and waste solvent treatment. Accordingly, we investigate the printing of donor-acceptor blend films out of different solvents for use as active layers in organic solar cells with advanced in-situ scattering methods. We use grazing incidence small and wide-angle X-ray scattering (GISAXS and GIWAXS) in-situ during printing to gain a fundamental understanding of the underlying film formation processes. Different examples of polymer donors and small molecule acceptors are presented, and the resulting morphologies are correlated with solar cell device performance. A special emphasis is put on the shift towards more environmentally friendly solvents, which will also be a prerequisite to promote the large-scale production of organic solar cells.

CPP 3.4 Mon 10:15 H38

The Role of Oxygen Insertion on Performance of A-D-A-type Non-Fullerene Acceptors (NFA) in Organic Solar Cells — •Wejdan Althobaiti[1], Yakun He[1], Julien Gorenflot[1], Wisnu Hadmojo[1], Sandeep Sharma[1], Filip Aniés[1], Weimin Zhang[1], Shahidul Alam[1], George Harrison[1], Anirudh Sharma[1], Shadi Fatayer[1], Derya Baran[1], Iain McCulloch[2], Thomas Anthopoulos[1], Martin Heeney[1], and Frédéric Laquai[1] — [1]King Abdullah University of Science and Technology (KAUST), Saudi Arabia — [2]University of Oxford, UK

Charge transfer in OSCs can occur through two pathways: photo-induced electron transfer from the donor to the acceptor, controlled by the electron affinity (EA) offset, and photo-induced hole transfer from the acceptor to the donor, governed by the ionization energy (IE) offset. Here, we report the synthesis of a novel NFA coded TPTI-BT, whose properties were first predicted by computational chemistry before the material was synthesized. Despite the favorable properties for high device performance, TPTI-BT exhibited moderate device performance, in particular when compared with the structurally-related and efficient acceptor O-IDTBCN. In fact, the chemical structure of TPTI-BT is very similar to that of O-IDTBCN, it contains only two additional oxygen atoms in the donor core of the A-D-A-type acceptor backbone structure. Interestingly, this causes TPTI-BT to exhibit overall lower device performance. We present a comparative study of these two NFAs and elucidate the origin of the lower performance of the TPTI-BT caused by two additional oxygen atoms.

CPP 3.5 Mon 10:30 H38

Revealing the effect of solvent additive selectivity on morphology and formation kinetics in printed non-fullerene organic solar cells at ambient conditions — •Jinsheng Zhang and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 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) and 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-C3-4F as the acceptor and introduce two distinct solvent additives one with superior solubility for PBDB-T-2F compared to BTP-C3-4F, 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 3.6 Mon 10:45 H38

Locally Resolved Thermally Induced Degradation on PM6:Y6-based Organic Solar Cells — •Shahidul Alam[1,2], José P. Jurado[2], Biwajit Pal[2], Zhuo Xu[3,4], Aurelien D. Sokeng[3,4], Harald Hoppe[3,4], and Frédéric Laquai[1,2] — [1]Physical Chemistry and Spectroscopy of Energy Materials, Department of Chemistry, LMU Munich, Germany — [2]King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Kingdom of Saudi Arabia — [3]Laboratory of Organic and Macromolecular Chemistry (IOMC), FSU Jena, Germany — [4]Center for Energy and Environmental Chemistry Jena (CEEC Jena), FSU Jena, Germany

The commercialization of new photovoltaic technology is impeded by the degradation of organic photovoltaic devices caused by thermal factors. Therefore, it is crucial to have an in-depth awareness of the underlying causes of thermal device instability and to develop effective approaches to reduce its negative impacts. This study examines the thermal degradation of PM6:Y6 bulk heterojunction solar cells, which are currently considered at the forefront of organic solar cell technology. The investigation focuses on the effects of varying temperatures on the performance and locally resolved thermally induced impact of these solar cells. We report a comprehensive study probing the influence of thermal annealing of solar cells by the use of several advanced optoelectrical and imaging characterization techniques.

CPP 3.7 Mon 11:00 H38

Thermal degradation behavior of BTP-4F-12 based green-solvent organic solar cells — •Zerui Li^1, Jinsheng Zhang^1, Simon Wegener^1, Yingying Yan^1, Xiongzhuo Jiang^1, Kun Sun^1, Matthias Schwartzkopf^2, Sarathlal Koyiloth Vayalil^{2,3}, and Peter Müller-Buschbaum^1 — ^{1}TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — ^{2}Deutsches Elektronen-Synchrotron DESY, 22607, Hamburg, Germany — ^{3}Applied Sciences Cluster, University of Petroleum and Energy Studies UPES, Dehradun, Uttarakhand, 248007, India

Thermal degradation is inevitable for organic solar cells in real application conditions. The common research of thermal stability could only observe ex-situ conditions before and after heating and the device behavior during heating is missing, which is insufficient to the understanding of degradation mechanisms. Herein, a new observation aspect is realized to analyze the thermal degradation of BTP-4F-12 based green-solvent organic solar cells with the application of operando GIWAXS/GISAXS, which provides a deep learning of thermal degradation. The OSC devices show a harsh Voc loss with temperature increase, which would recover mostly after getting cooled down to low temperature, while the loss of FF and Jsc during aging is irreversible. Thus, polymer donors play a crucial role in the device performance as well as thermal behavior. In addition, such thermal degradation is driven by the evolution of the molecular stacking and aggregation and thermal expansion/contraction during aging.

CPP 4: Crystallization, Nucleation and Self-Assembly I

Time: Monday 11:30–13:00 Location: H34

CPP 4.1 Mon 11:30 H34

Confined crystallization for studying kinetics and crystal orientation of interface-induced polymer crystallization — •Marthinus van Niekerk, Thomas Thurn-Albrecht, and Oleksandr Dolynchuk — Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Germany

Understanding interfacial interactions is essential to understanding the mechanisms and kinetics of interface-induced crystallization (IIC), namely heterogeneous nucleation or prefreezing, and resultant material properties. While heterogeneous nucleation is an activated process occurring below T_m, prefreezing is an equilibrium process producing a stable crystalline layer above T_m that thickens upon cooling. Quantifying the influence of interfacial interactions on the kinetics of IIC and crystal morphology has long been elusive and is addressed in this work. We present a systematic study of confined crystallization in micrometer-sized dewetted droplets of poly(ϵ-caprolactone) (PCL) on a range of substrates, allowing numerical analysis of isolated nucleation events and kinetics. Our results show that prefreezing significantly enhances crystallization kinetics compared to nucleation, resulting in simultaneous crystallization of PCL droplets close to T_m. X-ray scattering reveals the preferred crystal orientation in PCL droplets crystallized by IIC, which is strongest for prefreezing and is supported by striking differences in lamellar morphologies observed in AFM. Thus, we present both quantified nucleation kinetics and crystal orientation for different cases of IIC and show that prefreezing enhances crystallization kinetics and anisotropic crystal orientation most effectively.

CPP 4.2 Mon 11:45 H34

Liquid crystalline ordering of conjugated polymers at the vacuum interface — Anton Sinner, Alexander Johannes Much, and •Oleksandr Dolynchuk — Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Germany

Structure formation in films of conjugated polymers (CPs) strongly affects their optoelectronic properties and is of fundamental interest in the context of sanidic liquid crystalline (SLC) phases discovered in board-like polymers. Recent experimental results on films of the model CP poly(3-hexylthiophene) (P3HT) revealed the edge-on crystal orientation in the top film layer and suggested that the vacuum interface induces it. Here, we use grazing-incidence wide-angle X-ray scattering to study in situ the crystallization and melting in films of P3HT and polydiketopyrrolopyrrole (PDPP), another board-like CP, at the vacuum interface. Upon cooling from the melt, the ordering of both P3HT and PDPP indeed starts at the vacuum interface as an edge-on oriented disordered SLC phase and undergoes multiple SLC transitions with decreasing temperature. The same thermal hierarchy of SLC phases is observed for both CPs during melting, demonstrating that the vacuum interface stabilizes the edge-on disordered SLC phase above its bulk transition temperature, similar to the surface freezing of short alkanes. Notably, the observed effects are much stronger for PDPP, also resulting in a thicker edge-on oriented layer of more than 100 nm. Thus, we show that surface-induced SLC ordering is a general phenomenon of CPs, presumably due to their board-like architecture, and it significantly influences the molecular orientation in CP films.

CPP 4.3 Mon 12:00 H34

How Aqueous Solutions of Low-end Mono-alcohols Crystallize? — •Vasileios Moschos^1 and George Floudas^{1,2} — ^{1}Department of Physics, University of Ioannina, 45110 Ioannina, Greece — ^{2}Max Planck Institute for Polymer Research, 55128 Mainz, Germany

Aqueous solutions of low-end aliphatic mono-alcohols, such as ethanol and 1-propanol, display several peculiar features originating from hydrogen bonding, and in particular, antagonistic hydrophilic/hydrophobic interactions of the head/tail that give rise to local nano-heterogeneity. By combining structural (XRD), thermodynamic (Differential Scanning Calorimetry, DSC) and dynamical (Dielectric Spectroscopy, DS) probes, the pertinent phase diagrams of the two binary mixtures are established, comprising of liquid 1-propanol/ethanol, liquid water, hexagonal ice and different hydrates. The two phase diagrams are discussed in terms of up to five different Regimes (Regime I-V), all sharing a droplet arrangement of the minority component, with the exception of Regime I in ethanol/water binary system, where molecular mixing of the two components occurs. By probing the dynamics of the mixtures over an extended frequency and temperature range, different relaxation processes are identified, either associated with with the dynamics of pure alcohol (Debye-like and α-process) or alcohol/water mixtures.

CPP 4.4 Mon 12:15 H34

Intra-crystalline chain diffusion, semicrystalline morphology and mechanical modulus of selected aliphatic polyesters — •Qiang Yu, Albrecht Pezold, and Thomas Thurn-Albrecht — Martin-Luther-University Halle-Wittenberg

Aliphatic polyesters are good candidates to replace commodity plastics in many applications due to their similar mechanical and thermal properties, and superior degradability. However, their intra-crystalline chain diffusion (ICD, the mobility of polymer chains in the crystalline phase) and semicrystalline morphology have not been widely studied. From our recent studies, based on model polymers, semicrystalline polymers exhibit different morphological features depending on the timescale of ICD ($\langle\tau_c\rangle$) relative to the kinetics of crystal growth (τ_{lc}). To check the generality of the findings, our study is expanded into a series of A-B aliphatic polyesters. $\langle\tau_c\rangle$ and τ_{lc} of the polyesters were investigated by nuclear magnetic resonance (NMR) and polarized optical microscope, respectively. The semicrystalline morphology was monitored by small angle X-ray scattering (SAXS) during isothermal crystallization. Long $\langle\tau_c\rangle$ (not measurable by NMR) was qualitatively differentiated by different crystal thickening slopes (SAXS measurement). The results show that our findings are also valid for the investigated polyesters. The different crystal thickening slopes show that the ICD of polymers slows down due to the formation of layers of ester groups in the crystal. At last, we report on the exponential dependence of shear modulus of the polyesters with long $\langle\tau_c\rangle$ on their crystallinity.

CPP 4.5 Mon 12:30 H34

Self-assembled Peptides Structure Mediated by Solid Interfaces — •Leila Sahebmohammadi^1, Pol Besenius^2, Markus

Mezger[3], and Regine von Klitzing[1] — [1]Soft Matter at Interfaces, Department of Physics, Technical University of Darmstadt, Germany — [2]Department of Chemistry, Johannes Gutenberg-Universität Mainz, Germany — [3]Faculty of Physics, Universität Wien, Austria

The self-assembly of amphiphilic, C3-symmetric dendritic peptides is driven by non-covalent interactions and steric limitations. This study focuses on peptides with a thermosensitive moiety. In phosphate buffer, oppositely charged peptide amphiphiles form 1D nanorod-like patterns, confirmed by circular dichroism spectroscopy to follow a ß-sheet structure. Atomic Force Microscopy (AFM) revealed temperature-dependent helical filaments, where higher temperatures increased filament length and pitch due to the hydrophobic thermosensitive moiety, while reducing filament height. Quartz Crystal Microbalance with Dissipation (QCM-D) showed a temperature-responsive, layer-by-layer adsorption process forming stable multilayers. Lysine-based cationic comonomers improved adsorption and coating uniformity on gold (Au) and silicon (Si) surfaces. Extreme pH conditions (2 or 12) caused multilayer removal, revealing a pH-responsive mechanism from weakened electrostatic interactions. This study demonstrates how self-assembly and surface confinement adapt peptide assembly, offering insights for modifying surface properties for diverse applications.

CPP 4.6 Mon 12:45 H34

Crystallization and Pseudo-Isodimorphism in Statistical Copolythiophenes — •Alexander Johannes Much[1], Jakob Boris Günther Danziger[1], Qian Wang[2], Michael Sommer[2], and Oleksandr Dolynchuk[1] — [1]Martin-Luther-Universität Halle-Wittenberg — [2]Technische Universität Chemnitz

Statistical copolymerization is a powerful and widely used way to tailor material properties like solubility or mechanical properties. The copolymer properties depend largely on their co-crystallization and the crystal structure formed, which has been studied for polyesters, polyamides, and polycarbonates. The results suggest three co-crystallization scenarios: (1) total exclusion of comonomers, (2) total inclusion of comonomers (isomorphism), and (3) partial inclusion of comonomers into two crystal lattices (isodimorphism).

Here we study the co-crystallization and crystal structure of poly-(3-hexylthiophene)-stat-poly-[3-(6-cyanohexyl)thiophene] statistical copolymers using differential scanning calorimetry (DSC) and wide-angle X-ray scattering (WAXS). The composition-dependent melting temperatures and enthalpies obtained from DSC show minima, which is typical of isodimorphic co-crystallization. However, WAXS clearly indicates single crystal lattices in all copolymers, with a monotonic dependence of lattice constants on composition. This finding is inconsistent with isodimorphism, making the co-crystallization of these statistical copolythiophenes only pseudo-isodimorphic. Hence, our results suggest that the current classification of statistical copolymer crystallization is incomplete and needs to be extended.

CPP 5: Composites and Functional Polymer Hybrids

Time: Monday 11:30–13:00 Location: H38

Invited Talk CPP 5.1 Mon 11:30 H38

Theoretical characterization of sulfur/carbon copolymer cathodes for next-generation batteries via *ab initio* spectroscopy simulations — •Daniel Sebastiani and Pouya Partovi-Azar — Martin Luther University Halle-Wittenberg, Halle (Saale), Germany

The remarkable theoretical specific capacity of elemental sulfur (∼1675 mAh/g) and its abundance make lithium-sulfur (Li-S) batteries an attractive alternative to current lithium-ion technology. Nevertheless, their cycle life has so far been limited due to an irreversible capacity fade. To tackle this issue, numerous studies have focused on structural optimization of sulfur cathodes including utilization of sulfur/carbon copolymers. Among others, sulfur-n-1,3-diisopropenylbenzene (S/DIB) copolymer, a 3D network of DIB molecules interconnected via sulfur chains, has shown a promising performance as an active cathode material.

In this talk, we will present our recent works employing a quantum-chemical approach for the characterization of S/DIB copolymer cathodes through simulation of their Raman fingerprints during discharge. Theoretically predicted Raman responses, calculated at density-functional theory (DFT) level along with DFT-based *ab initio* molecular dynamics simulations, hint at activities at certain frequencies which can be exploited to experimentally distinguish between the underlying structures involving short or those having longer sulfur chains. These predictions are all proven plausible by experimental Raman measurements on Li-S coin cells.

CPP 5.2 Mon 12:00 H38

Unveiling the Kinetics of Block Copolymer Micelles Close Packing by In Situ GISAXS — •Guangjiu Pan[1], Jinsheng Zhang[1], Altantulga Buyan-Arivjikh[1], Zhuijun Xu[1], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]DESY, 22607 Hamburg, Germany — [3]KTH Royal Institute of Technology, SE 100 44 Stockholm, Sweden

Packing spheres has long been a key topic in science. While hard spheres often form dense, close-packed structures like face-centered cubic (FCC) lattices, soft spheres, such as block copolymers in selective solvents, tend to arrange into less dense structures. However, when using block copolymer templates in the sol-gel method, these soft spheres can achieve close-packed structures. In this study, in situ grazing-incidence small-angle X-ray scattering (GISAXS) is used to examine the self-assembly and co-assembly processes during the formation of close-packing structures. The results reveal that the hybrid films preferentially develop an FCC structure with cluster nuclei. After the polymer template is removed, a superlattice-like mesoporous metal oxide film is obtained, showcasing the potential for advanced applications due to its well-organized nanostructures.

CPP 5.3 Mon 12:15 H38

Optimizing the internal structure of soft elastic composite materials — •Lukas Fischer and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

We study magnetic gels and elastomers, soft materials composed of magnetic or magnetizable particles embedded in a soft polymeric matrix material. These materials can be controlled by external magnetic fields, which induce deformations (magnetostriction) or changes in the rheological behavior (magnetorheological effect).

In particular, we investigate how these two effects depend on the arrangement of magnetizable particles within the elastic matrix. For the magnetostrictive effect, we consider model systems of spherical shape, for which we can analytically calculate how the volume change and overall elongation or contraction under applied magnetic fields depends on the configuration (within the linear elastic regime) [1]. Based on these formulae, we optimize the structures for maximized deformations, using an adaption of simulated annealing. Additionally, we investigate cubical systems for their magnetorheological effects, also presenting the internal arrangements that maximize these effects. The optimized arrangements are compared to regular lattice configurations.

The method that we present here can be transferred to the investigation of other types of soft elastic composite systems, driving them towards their full potential in light of future applications.

[1] L. Fischer, A. M. Menzel, PNAS Nexus **3**, pgae353 (2024).

CPP 5.4 Mon 12:30 H38

Water dynamics in conductive PEDOT:PSS/cellulose nanocomposite films in dependence of relative humidity — •Lucas P. Kreuzer[1], Marie Betker[2], Marcell Wolf[1], Daniel Söderberg[3], and Stephan Roth[2,3] — [1]Heinz Maier-Leibnitz-Zentrum, Technische Universität München — [2]Deutsches Elektronen Synchrotron DESY — [3]Department of Fibre and Polymer Technlogy, KTH Royal Institute of Technology

Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) is a conductive polymer blend widely used in organic electronics. However, pure PEDOT:PSS films absorb significant amounts of water (≈50 V%), causing swelling, degradation, and eventually a decrease in conductivity. Integrating PEDOT:PSS with cellulose nanofibrils (CNFs) overcomes these issues by limiting water absorption and enhancing mechanical stability. However, in humid environments, a minor amount of water is still absorbed, leading to a change in film morphology: the absorbed water induces de-wetting of PEDOT:PSS from the CNFs, reducing conductivity, whereas drying generally leads to a re-wetting of PEDOT:PSS, thereby restoring conductivity. To investigate further the role of water, quasi-elastic neutron scattering is applied, which reveals two water species in the films: mobile bulk water and slower hydration water. Upon drying, bulk water is released completely, while hydration water remains in the films, supporting the re-wetting of PEDOT:PSS. QENS also provides information on the diffusive and hydrogen-bonding behavior of water.

CPP 5.5 Mon 12:45 H38

Enhanced Physical Properties and Shape Recovery in Epoxy-Based Shape Memory Polymer Nanocomposites under Gamma Irradiation for Aerospace Applications — •Eman Taha — 1 Ahmed El-Zomor St, 11727, Cairo, Egypt.

This research explores the impact of gamma irradiation on the structural and functional properties of epoxy-based shape memory polymer nanocomposites, specifically engineered for potential satellite deployment mechanisms in space applications. To enhance durability and adaptability in extreme conditions, multi-walled carbon nanotubes (MWCNTs) were incorporated into the epoxy matrix, with surfactants added to improve dispersion. Using a Cobalt-60 gamma irradiation facility, doses ranging from 250 to 1000 kGy were applied, uncovering dose-dependent changes in thermal stability and mechanical properties. Surface tension tests confirmed effective dispersion with nonionic (Tween 80) and anionic (SDS) surfactants, while cationic surfactants had less impact. Thermogravimetric analysis revealed enhanced thermal stability at moderate doses due to increased crosslinking. Dynamic mechanical analysis showed shifts in viscoelastic behavior and higher glass transition temperatures (Tg), critical for thermal stress resistance. Shape memory performance improved at 250 kGy but declined at higher doses, indicating a balance between radiation exposure and functionality. These findings highlight controlled gamma irradiation as a tool to optimize the performance and stability of epoxy-based nanocomposites with MWCNT reinforcement, advancing their suitability for space applications.

CPP 6: Gels, Polymers Networks and Elastomers II

Time: Monday 15:00–16:00 Location: H34

CPP 6.1 Mon 15:00 H34

Scattering data of A_4B_4 model networks reveal structure induced apparent interaction and cross-link repulsion — •Reinhard Scholz and Michael Lang — Leibniz-Institut für Polymerforschung, Hohe Str. 6, 01069 Dresden, Germany

Based on computer simulations, we analyze how different forms of labeling the network components allow to extract complementary structural information from scattering data. The analysis relies upon simulations of hetero-complementary bound four-functional star polymers A_4 and B_4. For optimized contrast between A and B stars, the calculated dynamic scattering intensity resembles A-B block copolymers with an apparent repulsion between both components, accounting for ordering effects due to the complementary coupling scheme. The position of the observed scattering peak is compatible with radius of gyration and end-to-end extension of A-B chains connecting adjacent star centers, providing access to the mesh size of the network. In samples with optimum contrast, the static correlation length Ξ is in the same range but somewhat smaller than the respective correlation length for homogeneously labeled polymers. Choices of the scattering contrast focusing on the star centers or on small regions around these reveal a correlation hole. Accordingly, scattering is suppressed towards small wave vectors, allowing for a decomposition of the observed scattering intensity into a product of the form factor of the labeled star sections and a structure factor describing the distribution of cross-links in space.

CPP 6.2 Mon 15:15 H34

Responsive Microgel Based Membranes — •Thomas Hellweg — Universität Bielefeld, Fak. f. Chemie, Physikalische und Biophysikalische Chemie, Universitätsstr. 25, 33615 Bielefeld

If microgels are made with comonomers which can act as (photo-)crosslinkable secondary crosslinker, they can be deposited in thin layers and subsequently be cross- linked by irradiation [1, 2]. Upon crosslinking freestanding membranes are obtained, which still exhibit the temperature response of the original microgels. The present contribution describes the synthesis and properties of the respective microgels, the membrane formation, and the membrane properties. The thermal response of the obtained 2D materials can be exploited to make gating membranes [3] which modulate ion flow by changing temperature which can be used in electrochemical devices. The resistance is found to steeply increase by up to an order of magnitude at the volume transition of the original microgels. Hence, these freestanding microgel membranes might be useful for building self- regulating fuel cells. Moreover, they can be doped with metal nanoparticles granting them catalytic activity and allowing to use them in flow reactors or microfluidic cells for chemical conversion [4].

[1] M. Dirksen, et al., Langmuir 2022, 38, 638-651.
[2] M. Dirksen, et al., RSC Adv., 2021, 11, 22014.
[3] S. Uredat, et al. , Phys. Chem. Chem. Phys. 2024, 26, 2732-2744
[4] V. Sabadasch, et al., ACS Applied Materials & Interfaces , 2022, 14, 43, 49181.

CPP 6.3 Mon 15:30 H34

Correlation between swelling ability, softness and adhesion of PNIPAM microgels — •Carina Schneider, Kevin Hagmann, Joanne Zimmer, Franziska Braun, and Regine von Klitzing — Departement of Physics, TU Darmstadt, Hochschulstraße 8, 64289, Darmstadt

PNIPAM microgels (poly-N-isopropylacrylamide) are polymeric cross-linked networks with a core-shell structure. Due to their volume phase transition, it is possible to control their swelling and mechanical behavior. However, the concept of softness in these microgels, is highly complex and is not a single, well-defined property. In this study we show that it rather has a multifold characteristic that arises from a combination of several factors, such as their (de-)swelling ability, mechanical properties and adsorption behavior at interfaces. The cross-linker density of the microgels affect their adsorption behavior at interfaces and faceting. For exploring the multifold softness of adsorbed PNIPAM microgels, atomic force microscopy (AFM) is used to directly probe the mechanical and adhesion properties through indentation measurements and related them to their swelling ability. These insights into the microgel behavior could inform the design of next-generation microgels for biomedical applications.

CPP 6.4 Mon 15:45 H34

Deformation and actuation of 3D-printed polymeric microstructures predicted by finite element simulations — •Santiago Gomez Melo and Ulrich Schwarz — Univesität Heidelberg, Heidelberg

Mechanical metamaterials with promising properties can be manufactured via 3D-printing of polymers. Computational modelling, in addition to aiding conceptualization and characterization, opens the gate towards computer rationalized material design. We present two projects to this end. First, we discuss the experimental investigation of 3D-printed tetrahedral polymeric microlattices with X-ray nanotomography. Step-wise loading and image processing allowed us to evaluate the evolution of the displacement fields. Finite element simulations were used to understand the strain accumulation around lattice defects. Second, we demonstrate that the thermomechanical response of printed nematic elastomer microstructures can be controlled via confinement in PDMS-scaffolds. We applied Landau-de Gennes theory combined with nonlinear morphoelasticity to predict the molecular orientation from the scaffold geometry and the actuation upon heating, in excellent agreement with experimental measurements of birefringence patterns.

CPP 7: Active Matter II (joint session BP/CPP/DY)

Time: Monday 15:00–17:00 Location: H37

CPP 7.1 Mon 15:00 H37

Emerging cellular dynamics from turbulent flows steered by active filaments — Mehrana Nejad[1,4], Julia Yeomans[2], and •Sumesh Thampi[2,3] — [1]Department of Physics, Harvard University, Cambridge, MA 02138 — [2]The Rudolf Peierls Centre for Theoretical Physics, Parks Road, Oxford OX1 3PU, UK — [3]Department of Chemical Engineering, Indian Institute of Technology, Madras, Chennai, India 600036 — [4]School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA

Describing the mechanics of cell collectives and tissues within the framework of active matter, without resorting to the details of biology is an exciting area. We develop a continuum theory to describe the dynamics of cellular collectives, discerning the cellular force-generating active filaments from cells shape. The theory shows that active flows and straining part of the active turbulence can elongate isotropic cells, which form nematic domains. This is important as cell morphology is not only an indicator of diseases but it can affect the nucleus morphology, gene expression and other biochemical processes inside the cells. Our theory highlights the importance of distinguishing the roles of active filaments from cell shape and explains outstanding experimental observations such as the origin of cell-filament alignment patches. Further, we reconcile how the contractile forces generated by the cytoskeletal network makes the cells to exhibit flow behaviours similar to that of extensile active systems. Revealing the crucial role of activity and rheology to describe the dynamics of cellular layers, our study is in consonance with a number of experimental observations.

CPP 7.2 Mon 15:15 H37

Defects in active solids: self-propulsion without flow — •Fridtjof Brauns[1], Myles O'Leary[2], Arthur Hernandez[3], Mark Bowick[1], and Cristina Marchetti[4] — [1]Kavli Institute for Theoretical Physics, Santa Barbara, USA — [2]Princeton University, Princeton, USA — [3]Leiden University, Leiden, the Netherlands — [4]University of California Santa Barbara, Santa Barbara, California 93106, USA

Topological defects are a key feature of orientational order and act as organizing centers of orientation fields. Self-propulsion of $+1/2$ defects has been extensively studied in active nematic fluids, where the defects are advected with the fluid through the flow field they generate. Here, we propose a minimal model for defect self-propulsion in a nematic active solid: a linear elastic medium with an embedded nematic texture that generates active stress and in turn is coupled to elastic strain. We show that such coupling gives rise to self-propelled $+1/2$ defects that move relative to the elastic medium by local remodeling of the nematic texture. This mechanism is fundamentally different from the fluid case. We show that this mechanism can lead to unbinding of defect pairs and stabilize $+1$ defects. Our findings might help explain how orientational order, e.g. of muscle fibers, is reconfigured during morphogenesis in solid-like tissues. For instance, motility and merging of $+1/2$ defects play a crucial role in setting up the body axis during Hydra regeneration.

CPP 7.3 Mon 15:30 H37

Isovolumetric dividing active matter — Samantha R. Lish[1], Lukas Hupe[1], Ramin Golestanian[1,2], and •Philip Bittihn[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

We introduce and theoretically investigate a minimal particle-based model for a new class of active matter where particles exhibit directional, volume-conserving division in confinement while interacting sterically, mimicking cells in early embryogenesis. We find that complex motion, synchronized within division cycles, displays strong collective effects and becomes self-similar in the long-time limit. Introducing the method of normalized retraced trajectories, we show that the transgenerational motion caused by cell division can be mapped to a time-inhomogenous random walk with an exponentially decreasing length scale. Analytical predictions for this stochastic process allow us to extract effective parameters, indicating unusual effects of crowding and absence of jamming. Robustness of our findings against desynchronized divisions, cell size dispersity, and variations in confinement hints at universal behavior. Our results establish an understanding of the complex dynamics exhibited by isovolumetric division over long timescales, paving the way for new bioengineering strategies and perspectives on living matter.

CPP 7.4 Mon 15:45 H37

Tracking plankton-to-biofilm transition in phototrophic bacteria — •Anupam Sengupta — Physics of Living Matter Group, Department of Physics and Materials Science, University of Luxembourg, Luxembourg — Institute for Advanced Studies, University of Luxembourg, Luxembourg

Phototrophic bacteria commonly inhabit natural aquatic and marine ecosystems, exhibiting both motile and sessile lifestyles [1]. Yet, how and when they switch between the two states has remained unknown. Using quantitative imaging, AFM and mathematical modeling, we track the conditions and phenotypic changes across multiple generations in Chromatium okenii, a motile phototrophic purple sulfur bacterium [2]. Enhanced cell-surface adhesion together with changes in the cell shape and cellular mass distribution facilitate the motile-to-sessile shift. Our results, supported by cell mechanics model, establish a synergistic link between motility, mass distribution and surface attachment in promoting biofilm lifestyle. [1] T. Sommer et al., Geophys. Res. Lett. 44, 2017. [2] F. Di Nezio,.., & A. Sengupta, Plos one 19, e0310265, 2024.

15 min. break

CPP 7.5 Mon 16:15 H37

How localized active noises influence the conformations and dynamics of semiflexible filaments — •Shashank Ravichandir[1], Jens-Uwe Sommer[1,2], and Abhinav Sharma[1,3] — [1]Leibniz-Institut für Polymerforschung, 01069 Dresden, Germany — [2]Technische Universität Dresden, 01069 Dresden, Germany — [3]Universität Augsburg, 86159 Augsburg, Germany

The structure and dynamics of active polymers have been recently studied in some detail. In these works all the monomers are considered to be active. However, in most biological systems non-equilibrium fluctuations manifest as activity only at isolated locations within the polymer. There have been only few studies of such polymers, in which the active monomers occur periodically along the polymer contour. We consider arbitrary active-passive copolymers and isolate the effects of the number and locations of active monomers on the conformational and dynamical properties of polymers. We use Langevin dynamics simulations to calculate the end-to-end distance, radius of gyration, and mean-squared displacement of such semiflexible filaments and classify the various states of these polymers based on their conformational properties. We also present preliminary results of polymers in which the location of active monomer moves dynamically along the chain contour. This is an idealized model of biopolymers such as DNA, during DNA transcription, and microtubules, which are driven by kinetic motors that traverse along its length.

CPP 7.6 Mon 16:30 H37

Sequence-specific folding of partially active polymers — •Shibananda Das — Department of Physics, Indian Institute of Science, Bengaluru, India

Biological polymers like actin filaments and microtubules exhibit important physical properties due to their out-of-equilibrium behavior induced by ATP or GTP. In contrast, synthetic polymers rely on energy from their surrounding environment, often using local chemical, electrical, or thermal gradients to remain far from equilibrium. Theoretically, active polymers serve as minimal models for these systems, enabling systematic study of the competition between thermodynamic and active forces while they undergo conformational changes.

Using a combined analytical and numerical approach, we investigate an active polymeric chain composed of multiple self-avoiding units, representing good solvent condition in the absence of active forces. For partially active polymers without orientational constraints, we find that distribution of the active units in distinct sequences along the backbone can induce a significant collapse into folded, globular structures. Detailed analysis shows that this activity-dependent collapse is driven by a reduction in swim pressure of the monomers, linking the distribution of active forces along the polymer contour to its folded conformations.

CPP 7.7 Mon 16:45 H37

Effect of interactions on the chemotactic response of active-passive chains — •Hossein Vahid[1], Jens-Uwe Sommer[1,2], and Abhinav Sharma[3] — [1]Leibniz-Institut für Polymerforschung, Dresden, Germany — [2]Technische Universität Dresden, Germany — [3]University of Augsburg, Augsburg, Germany

Living organisms, from single cells to populations, exhibit complex behaviors driven by the need to navigate toward favorable environments. These behaviors are often shaped by interactions within clusters or mixed populations, where collective dynamics play a crucial role in the characteristic properties of multicellular systems.

Chemotactic bacteria, found in diverse environments such as the gastrointestinal tract, plant surfaces, and aquatic ecosystems, demonstrate the significance of chemotaxis at the population level. While extensive research has focused on the properties of active polymers in spatially homogeneous activity fields, their behaviors in inhomogeneous fields remain less explored.

This study investigates the behavior of self-propelled polymers in activity gradients, emphasizing the effects of inter- and intra-chain interactions, such as steric and excluded volume effects, on chemotactic responses. These interactions give rise to distinct phases or collective behaviors that influence the stability and persistence of chemotaxis. Additionally, polymer density emerges as a critical factor impacting diffusion and the overall efficiency of chemotaxis. This work aims to study the dynamics of the active polymer populations in non-uniform environments systematically.

CPP 8: Hybrid and Perovskite Photovoltaics I

Time: Monday 15:00–16:00 Location: H38

Invited Talk CPP 8.1 Mon 15:00 H38

The Nanoscale Photovoltaics Laboratory on a Tip — •Stefan Weber — Institute for Photovoltaics, University of Stuttgart — Max Planck Institute for Polymer Research

Electrical scanning probe microscopy (SPM) modes are ideal for nanoscale photovoltaic measurements. I will discuss our recent work on developing specialized SPM techniques to study hybrid perovskite materials. Optimizing perovskite solar cells requires understanding energy losses, instability, and aging processes. These macroscale properties result from the interplay between nanoscale structure and function, including twin domains, grain boundaries, interfaces, and crystal grain orientations. Using static and time-resolved Kelvin probe force microscopy (KPFM), we can map the local surface potential, surface photovoltage (SPV), and cross-sectional potential distributions under operating conditions. With Nano-SPV spectroscopy, we achieve 10-20 nm lateral- and sub-millisecond temporal resolution. Our research aims to address key challenges in perovskite research, such as phase segregation, degradation, and interface heterogeneity, advancing understanding of loss mechanisms and instabilities in MHP solar cells.

CPP 8.2 Mon 15:30 H38

Sputter-Deposited TiOx Thin Film as a Buried Interface Modification Layer for Efficient and Stable Perovskite Solar Cells — •Xiongzhuo Jiang[1], Kun Sun[1], Zerui Li[1], Zhuijun Xu[1], Guangjiu Pan[1], Yusuf Bulut[1,2], Benedikt Sochor[2], Matthias Schwartzkopf[2], Kristian A. Reck[3], Thomas Strunskus[3], Franz Faupel[3], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [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

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. Herein, TiO_x layers are deposited onto a SnO_2 layer via sputter deposition at room temperature, forming a bilayer HBL. The structure evolution of TiO_x during sputter deposition is investigated via in situ grazing-incidence small-angle X-ray scattering. After sputter deposition of TiO_x with a suitable thickness on the SnO_2 layer, the bilayer HBL 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 SnO_2/TiO_x functional bilayer, the perovskite solar cells exhibit higher power conversion efficiencies than the unmodified SnO_2 monolayer devices.

CPP 8.3 Mon 15:45 H38

Dynamics and kinetics of light-induced phase segregation in $MAPbBr_{1.8}I_{1.2}$ perovskites — •Ivan Zaluzhnyy[1], Linus Pithan[2], Rustam Rysov[2], Frederik Unger[1,2], Jakub Hagara[1], Ekaterina Kneschaurek[1], Paul Zimmermann[1], Sebastian Schwartzkopff[1], Lena Merten[1], Dmitry Lapkin[1], Alexander Hinderhofer[1], Fabian Westermeier[2], Michael Sprung[2], Yana Vaynzof[3,4], Fabian Paulus[5,4], and Frank Schreiber[1] — [1]University of Tübingen — [2]Deutsches Elektronen-Synchrotron DESY — [3]Technical University of Dresden — [4]Center for Advancing Electronics Dresden (cfaed) — [5]IFW Dresden

Hybrid organic-inorganic perovskites tend to undergo several structural transformations that can be caused by temperature, humidity and light. Here we use X-ray photon correlation spectroscopy (XPCS) to study the dynamics of light-induced phase segregation in $MAPbBr_{1.8}I_{1.2}$ and the formation of Br-rich and I-rich domains. We observe that the phase segregation is characterized by three distinct time scales corresponding to the rapid formation of small seeds of the I-rich phase, fluctuations of the ion distribution around the quasi-equilibrium state (dynamics), and a directional drift of the ions within the crystal grains (kinetics). We also observe the influence of defects in the halide sublattice on phase separation and find that samples with interstitial halides exhibit slower phase separation as samples with vacancies in the halide sublattice.

CPP 9: Biomaterials and Biopolymers (joint session BP/CPP)

Time: Monday 15:00–16:45 Location: H46

CPP 9.1 Mon 15:00 H46

Ferroelectric Microelectrodes for Hybrid Neuroelectronic Systems — •Maximilian T. Becker[1,2], Roland Thewes[3], and Günther Zeck[4] — [1]Department of Embedded Systems, Hahn-Schickard, Freiburg, Germany — [2]Faculty of Engineering, University of Freiburg, Freiburg, Germany — [3]Chair of Sensor and Actuator Systems, TU Berlin, Berlin, Germany — [4]Institute of Biomedical Electronics, TU Wien, Vienna, Austria

Direct electrical interfacing of semiconductor chips with individual neurons and neural networks forms the basis for a systematic assembly and investigation of hybrid neuroelectronic systems with future applications in information technology and biomedicine. The neuroelectronic interface is realized via microelectrodes to bidirectionally transmit electrical signals between neurons and the semiconductor chip. Here, we introduce the concept of ferroelectric microelectrodes and discuss the physics of ferroelectric interfaces in neuroelectronic applications. As an example, we present neural recordings from retinal ganglion cells (RGCs) interfaced with a ferroelectric complementary metal-oxide-semiconductor microelectrode array (CMOS-MEA) and discuss the results in detail.

CPP 9.2 Mon 15:15 H46

Highly sensitive, specific and label-free detection of SARS-CoV-2, Influenza A and RSV proteins via surface plasmon resonance technique using the biofunctionalization with 1 nm thick carbon nanomembranes — •Ghazaleh Eshaghi[1], David Kaiser[1], Hamid Reza Rasouli[1], Rania Ennaciri[1], Martha Frey[1], Christof Neumann[1], Dominik Gary[2], Tobias Fischer[2], Katrin Frankenfeld[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Forschungszentrum für Medizintechnik und Biotechnologie (fzmb) GmbH, 99947 Bad Langensalza, Germany

Accurate and rapid detection of respiratory viruses like SARS-CoV-2, Influenza A and RSV is crucial for improving global health outcomes. We present a novel surface plasmon resonance (SPR) platform using a biofunctionalized 1 nm-thick carbon nanomembrane (CNM) for enhanced viral protein detection. The azide-modified CNM (N3-CNM) enables covalent antibody binding, ensuring selective immobilization of target proteins. Our platform achieves equilibrium dissociation constants (KD) of 570 * 30 pM and 22 * 3 pM for SARS-CoV-2 nucleocapsid and spike proteins, with detection limits (LODs) of ~190 pM and ~10 pM, respectively. For Influenza A and RSV, KD values are 86 * 4 pM and 3 * 0.2 pM, with LODs of ~90 pM and ~2 pM. Multiplexed detection with no cross-reactivity supports rapid, accurate point-of-care diagnostics. Validation with nasopharyngeal swabs confirms a LOD of ~40 pM for SARS-CoV-2 spike protein, highlighting CNMs' promise in infectious disease diagnostics.

CPP 9.3 Mon 15:30 H46

Superselective multivalent client recruitment in biomolecular condensates — •Xiuyang Xia and Erwin Frey — Ludwig-Maximilians-Universität München

Biomolecular condensates (BMCs) are membraneless organelles formed via liquid-liquid phase separation, playing a crucial role in organizing cellular functions by selectively concentrating specific molecules. In this talk, I will present a new theoretical framework that models multivalent client recruitment in valence-limited, multicomponent systems like BMCs. We uncover how enthalpic and entropic factors interplay under valence constraints to enable switch-like recruitment and precise compositional regulation.

This work advances our understanding of the principles governing BMC composition and highlights the broader significance of multivalency in biological systems, offering insights into cellular organization and potential therapeutic applications.

CPP 9.4 Mon 15:45 H46

What is the structure of a biomolecular condensate? — •Charlotta Lorenz[1,2], Teagan Bate[1], Takumi Matsuzawa[1], Kaarthik Varma[1], Sully Bailey-Darland[1], George Wang[1], Dana Matthias[1], Harsha Koganti[2], Nicola Galvanetto[2], Matti Valdimarsson[2], Aleksander Rebane[3], Etienne Jambon-Puillet[4], Ben Schuler[2], and Eric R. Dufresne[1] — [1]Cornell University, Ithaca, NY, USA — [2]University of Zurich, Zurich, Switzerland — [3]New York University Abu Dhabi, Abu Dhabi, United Arab Emirates — [4]École Polytechnique Paris, Paris, France

Biomolecular condensates are important for a variety of cellular functions, such as biochemical regulation, structural organization, and RNA metabolism. While the properties and physiology of these condensates depend on their structure, this important aspect has received little experimental consideration. On the other hand, recent simulations of disordered proteins with interactions based on the sticker-and-spacer suggest fascinating structures in the bulk and surface of condensates. We aim to reveal the structure of biomolecular condensates using X-ray scattering. Here, we will present results for a simple model system and apply our approach to the structure of condensates made of disordered proteins. We particularly consider the change in condensate structure due to small molecules.

CPP 9.5 Mon 16:00 H46

Encoding how shear stress during gelation boosts the stiffness of collagen networks — •Pavlik Lettinga[1,2], Lens Dedroog[2], Olivier Deschaume[2], Yovan de Coene[2], Carmen Bartic[2], Erin Koos[2], and Mehdi Bouzid[3] — [1]Forschungszentrum Jülich — [2]KU Leuven — [3]Université Grenoble Alpes

Collagen is one of the main building blocks of the mammalian extracellular matrix, due to its ability to form tough structures with a wide variety of non-linear mechanical properties allowing it to support multiple tissue types. However, the mechanical properties of collagen gels have been extensively studied under static conditions, whereas in nature gelation will mostly take place in the presence of flow. Here we show how the elastic modulus of collagen hydrogels can be increased up to an order of magnitude by applying a stress ramp at a well-defined moment during gelation. Where the first stress block induces most of the final strain and alignment, sequential increases in stress cause a dramatic increase of the modulus. This high modulus is preserved by keeping the high stress until the gel is fully matured. Coarse-grained simulations of a model gel system show that that the microscopic mechanism of inducing high stiffness is due to formation of extra cross bridges and could be very generic. Thus, we not only show that the true non-linear capabilities of biomaterials are tenfold higher than previously assessed, but also provide insight into in vivo structure formation of collagen and potentially other (bio-)polymers.

Invited Talk CPP 9.6 Mon 16:15 H46

In situ control of cells and multicellular structures at the microscale by two-photon lithography — •Christine Selhuber-Unkel — Heidelberg University, IMSEAM, Heidelberg, Germany

In vivo, cells and multicellular assemblies often experience strong confinement by their surrounding tissue environment, particularly in cancer. Thus, replicating these confined environments in situ is essential for investigating their impact on cellular systems. Using two-photon lithography, we printed structures directly within and around multicellular assemblies. For example, we fabricated dome-shaped confinements with micrometer-scale openings to encapsulate cancer spheroids. This enabled us to study how confinement influences cancer cell migration and spheroid behavior. Our findings revealed that confinement slows cell migration and alters actin dynamics. In addition, in situ printed structures can also directly interfere with migrating cellular assemblies. Additionally, elastic structures can be created to mechanically stimulate cells, offering further control over cellular behavior. Therefore, two-photon lithography proves to be a powerful tool for manipulating the growth, migration, and morphology of live cells, making it particularly useful for exploring how changing physical microenvironment in situ affect cell responses.

CPP 10: Wetting, Fluidics and Liquids at Interfaces and Surfaces I (joint session CPP/DY)

Time: Monday 16:15–17:15 Location: H34

CPP 10.1 Mon 16:15 H34

Beyond contact angle measurements of aerophilic surfaces — •Alexander Tesler[1], Wolfgang Goldmann[1], Anca Mazare[2], Ben Fabry[1], Stefan Kolle[3], Robin A.H. Ras[4], Heikki Nurmi[4], George Sarau[5], and Silke Christiansen[5] — [1]Biophysics Chair, Erlangen, Germany — [2]WW4-LKO, Erlangen, Germany — [3]UCSD, San Diego, USA — [4]Aalto University, Epsoo, Finland — [5]Fraunhofer Institute, Forchheim, Germany

Aerophilicity can provide surface resilience to the detrimental effects of wetting-related phenomena. However, the development of such superhydrophobic surfaces with a long-lasting entrapped air layer, called plastron, is hampered by the lack of evaluation criteria and methods that can unambiguously distinguish between stable and metastable Cassie-Baxter wetting regimes. The information to evaluate the stability of the wetting regime is missing from the commonly used contact angle goniometry. Therefore, it is necessary to determine which surface features can be used as a signature to identify thermodynamically stable plastron. Here, I describe a methodology for evaluating the thermodynamic underwater stability of the Cassie-Baxter wetting regime of superhydrophobic surfaces by measuring the surface roughness, solid-liquid area fraction, and Young's contact angle. The method allowed the prediction of passive plastron stability for over one year of continuous submersion,[1] impeding mussel and barnacle adhesion,[2] and inhibition of metal corrosion in seawater.[3] [1] Tesler et al., Commun. Mater. 2024, 5, 112. [2] Tesler et al., Nat. Mater. 2023, 22, 1548. [3] Prado et al., Adv. Funct. Mater. 2024, 35, 2407444.

CPP 10.2 Mon 16:30 H34

Fluid flow inside slit-shaped nanopores: the role of molecular surface morphology — •Giorgia Marcelli[1], Tecla Bottinelli Montadon[1], Roya Ebrahimi Viand[1], and Felix Höfling[1,2] — [1]Institute of Mathematics, Freie Universität Berlin, Germany — [2]Zuse Institute Berlin, Germany

The boundary conditions of nanoscale flows near surfaces can deviate from the no-slip condition observed at macroscopic scales, and used in classical fluid mechanics. In this context, we investigate the influence of surface morphology on fluid flow inside slit-shaped nanopores [1]. Using non-equilibrium molecular dynamics (NEMD) simulations, we demonstrate that the surface morphology effectively controls the slip length, which approaches zero when the molecular structures of the pore wall and the fluid are matched. We examine two types of pore walls, mimicking a crystalline and an amorphous material, that exhibit markedly different surface resistances to flow. The resulting flow velocity profiles are consistent with Hagen–Poiseuille theory for incompressible, Newtonian fluids when adjusted for surface slip and effective viscosity; the latter is found to vary substantially with the pore width. Moreover, analysis of the hydrodynamic permeability shows that the simulated flows are in the Darcy regime. We further show that thermal isolation within the pore causes a linear increase in fluid temperature along the flow, which we relate to strong viscous dissipation and heat convection, utilizing the conservation laws of fluid mechanics.

[1] G. Marcelli, T. Bottinelli Montadon, R. Ebrahimi Viand, and F. Höfling, arXiv:2411.04882 [cond-mat.soft].

CPP 10.3 Mon 16:45 H34

How do polymers of different architecture penetrate nanochannels? — •Panagiotis Kardasis[1] and George Floudas[2] — [1]Department of Physics, University of Ioannina, 45110 Ioannina, Greece — [2]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

The way that polymers penetrate narrow pores is of both academic and technological importance. Capillary force can drag polymer chains into nanopores, a process called imbibition. Using in situ nanodielectric spectroscopy (nDS), we report the imbibition and following adsorption kinetics of star cis-1,4-polyisoprenes (SPI) and of bottlebrush polymers directly at the chain length scale by monitoring the evolution of the normal modes, during the flow within in alumina nanopores (AAO), as a function of chain architecture (vs linear), pore size, molar mass, and temperature. We demonstrate that the imbibition kinetics of SPIs proceeds via a slow adsorption mechanism, about 2 orders of magnitude slower than in linear polyisoprenes (PI). We further demonstrate that the bottlebrush topology results in slower adsorption in nanopores in comparison to linear counterpart, albeit, with different dependence. Additionally, bottlebrushes present weaker temperature dependence comparing to both linear and star polymers. Furthermore, we explore how symmetric star / linear and brush / linear blends penetrate the same nanopores and we demonstrate that differences in the imbibition and adsorption kinetics can be used to separate the homogeneous blend to its components, giving rise to *topology sorting*, based on the relative viscosities and pore diameter.

CPP 10.4 Mon 17:00 H34

Removing particles from hydrophobic surfaces by single water drops — •Franziska Sabath, Stefanie Kirschner, and Doris Vollmer — Max Planck Institute for Polymer Research, 55128 Mainz, Germany

The accumulation of dust on surfaces is a well-known phenomenon in everyday life, for example on windows and solar panels. Both manual cleaning and self-cleaning of hydrophobic surfaces with water can restore the properties of soiled surfaces. However, it is not yet understood how particles are removed by a water drop and which forces play a role for successfully removing the particles. We investigated the removal of two or more particles from hydrophobic coatings by a single water drop. For this purpose, we used a confocal microscope with a sliding drop setup. This implies that the particles was moved at constant velocity while the drop is hold in position by a blade. The sliding drop and the way in which the particles are picked up and pulled along by the water drop can be imaged. From the deflection of the blade, we can determine the force required to pull the particles along with the drop. Here, we focus on the removal of spherical model particles and the impact of drop volume, particles size and particle velocity on the particle removal. At low velocities the particles remain attached to the drop. With increasing velocity we observe that the particle detachment becomes more likely. In case of particle detachment, we observe a correlative effect: after the second particle has reached the rear side of the drop, both particles can detach together.

CPP 11: Hybrid and Perovskite Photovoltaics II

Time: Monday 16:15–17:00 Location: H38

CPP 11.1 Mon 16:15 H38

Structure and morphology investigations on slot-die coated perovskite nanocrystal films — •Thomas Baier[1], Altantulga Buyan-Arivjikh[1], Lixing Li[1], Xiaojing Ci[1], Matthias Schwartzkopf[2], Sarathlal Koyiloth Vayalil[2,3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Applied Sciences Cluster, University of Petroleum and Engergy Studies UPES, Dehradun, Uttarakhand 248007, India

Perovskite quantum nanocrystals hold great potential for contributing to the future renewable energy mix by serving as the active layer in solar cells. This potential arises from quantum confinement effects, which occur when crystal sizes are reduced below the Bohr radius. These nanocrystals achieve high power conversion efficiencies, excellent photoluminescence quantum yield (PLQY), narrow photoluminescence (PL) peaks, and enhanced stability compared to bulk perovskite. Additionally, the choice of X halides (I-, Br-, Cl-) and A-site cations (FA+, MA+, Cs+) within the ABX3 perovskite structure allows precise bandgap tuning. Cesium-formamidinium lead iodide perovskite nanocrystals have been prepared and slot-die coated. These perovskite nanocrystals as active layers are investigated using in-situ grazing incidence small- & wide-angle x-ray scattering (GISAXS & GIWAXS) to better understand the layers formation process.

CPP 11.2 Mon 16:30 H38

Tracking the Crystallization Pathway of Perovskite using Microscopy, Spectroscopy and Machine Learning — •Meike Kuhn[1], Milan Harth[2], Alessio Gagliardi[2], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]Simulation of Nanosystems for Energy Conversion, Technische Universität München, Hans-Piloty-Str. 1, 85748 Garching b. München, Germany

The interest in perovskite materials has grown significantly in recent years due to their diverse applications, with the crystallization process playing a crucial role in determining the final properties of perovskite films. Time-resolved techniques, such as microscopy and spectroscopy, enable detailed analysis of the various stages of perovskite formation.

In this study, we investigated the crystallization of methylammonium lead iodide (MAPbI3) blade coated from dimethylformamide (DMF), using a combined microscopy and spectroscopy approach. This approach allowed us to observe morphological and optical changes during intermediate phase formation and perovskite conversion, influenced by the addition of various additives. By applying a machine learning model to the microscopy data, we developed a predictive framework capable of estimating spectroscopic signals, thus enabling insights into physical properties with time-resolved microscopy.

CPP 11.3 Mon 16:45 H38

Utilizing CsPbBr3 Nanocrystals as Nucleation Seeds for Scalable FAPbI3 Thin Films — •Altantulga Buyan-Arivjikh[1], Jascha Fricker[1], Thomas Baier[1], Xiaojing Ci[1], Lixing Li[1], Matthias Schwartzkopf[2], Sarathlal Koyiloth Vayalil[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]DESY, 22604 Hamburg, 22607, Germany

Lead-halide perovskites have gained a significant 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, where the crystallinity and morphology of the thin film are critical factors influencing the properties and performance of perovskites. In this work, we present a novel approach for improving the quality of FAPbI3 thin films by utilizing CsPbBr3 nanocrystals as nucleation seeds. In-situ optical spectroscopy experiments reveal a faster transition of FAPbI3 into the photactive phase in the seeded thin films as well as a reduced defect density. In-situ grazing incidence wide angle X-ray scattering (GIWAXS) measurements confirm the former and additionally show that the seed crystals improve the thin film texture by inducing a preferred crystallite orientation.

CPP 12: Biomaterials, Biopolymers and Bioinspired Functional Materials I (joint session CPP/BP)

Time: Monday 17:00–18:00 Location: H46

CPP 12.1 Mon 17:00 H46

Polymer Assisted Condensation and Heterochromatin — •Jens-Uwe Sommer — Leibniz-Institut für Polymerforschung Dresden (IPF), Hohe Straße 6, 01069 Dresden, Germany — TU Dresden, Insitut für Theoretische Physik, Zellescher Weg 17, D-01069 Dresden, Germany

Many biomolecular condensates are formed through the co-condensation of proteins and polynucleotides. In most cases, the proteins that constitute the majority of the condensate exhibit a miscibility gap in aqueous solution at elevated concentrations in vitro. Recently, we published the theory of Polymer-Assisted Condensation (PAC), which predicts the formation of the condensate within the polymer's volume of gyration, where interactions with the three-dimensional conformation of the polymer trigger the phase transition of the protein component [1]. A key feature of these liquid condensates is their robustness against changes in parameters, as well as the dominant role played by the condensation free energy of the protein component. The formation and properties of heterochromatin, a genetically silenced region of eukaryotic chromosomes, can be explained by PAC, which resolves several issues present in previously published theories. Recently, we developed a field-theoretic approach to PAC to better understand the adsorption and desorption scenarios of heterochromatin at the nuclear lamina.

[1] J.-U. Sommer, H. Merlitz, and H. Schießel, Macromolecules 55, 4841 (2022); L. Haugk, H. Merlitz, and J.-U. Sommer, Macromolecules 57, 9476 (2024)

CPP 12.2 Mon 17:15 H46

How specific binding induces sol-gel transitions and liquid-liquid phase separation in RNA/protein solutions: Coarse-grained simulations versus Semenov-Rubinstein Theory — •Xinxiang Chen, Jude Ann Vishnu, Pol Besenius, Julian König, and Friederike Schmid — Johannes Gutenberg-University, Mainz, Germany

Liquid-liquid phase separation plays a central role in cellular organization, including RNA splicing. RNA-protein interactions are crucial to these processes. A key factor in controlling the phase behavior of RNA-protein systems is the sequence of binding and neutral domains. Using molecular dynamics simulations, we investigate phase transitions in RNA-protein solutions that are driven solely by specific binding interactions. The model omits nonspecific interactions including electrostatic interactions. We show that specific binding interactions induce a percolation transition with double reentrant behavior without phase separation, if the neutral linker size is long. Comparing our results with the two-component Rubinstein-Semenov theory, we find that the theory qualitatively reproduces the phase diagram of the percolation transition and the impact of the neutral domains. Phase separation is observed when reducing the neutral linker size in an asymmetric system, resulting in a closed-loop phase diagram. We also study the effect of modulating the sequence and find that blockiness of sticker sites introduces microstructure in the dense liquid phase. These insights enhance our understanding of how specific binding and domain arrangement regulates condensate formation in RNA-protein systems.

CPP 12.3 Mon 17:30 H46

Model particles to study interaction of microplastic particles

— •Kai Gossen, Andreas Fery, and Günter Auernhammer — IPF Dresden, Dresden, Germany

Microplastic in the environment is typically coated by natural organic matter forming an ecocorona. We present an approach to model ecocorona on particles with well-defined polymers, synthetic and derived from natural polymers. Polystyrene particles were coated with fluorescent polyelectrolyte multilayer systems, PS(Chitosan/Hyaluronic acid) and PS(Poly(dimethyldiallylammonium chloride) /Polystyrene sulfonate) by the layer-by-layer method. Systems with 2, 4 and 6 bilayers were synthesized. The second layers were fluorescently labelled with SNARF conjugated dextran.

It was found that zeta potentials of the PS(Chi/HS)2/4/6 systems assume values (-20 mV to -35 mV) that are similar to those of PS-ecocorona particles (-40 mV to -5 mV). The pH-dependent fluorescence of particle suspensions and individual particles were measured at pH values between pH 3 and pH 8. A well measurable pH dependence between pH 4.5 and 8 for the PS(Chi/HS) systems and the PS(PDADMAC/PSS) system could be measured. The system could serve to selectively study effects of surface properties of ecocorona coated particles such as surface stiffness or zeta potential.

CPP 12.4 Mon 17:45 H46

Microgels for Enhanced Adsorption of Endothelial Cells on Artificial Networks — •Souraj Mandal[1], Anna Fritschen[2], Alina Filatova[3], and Regine von Klitzing[1] — [1]Soft Matter at Interfaces, Department of Physics, Technical University of Darmstadt, Darmstadt 64289, Germany — [2]BioMedical Printing Technology, Department of Mechanical Engineering, Technical University of Darmstadt, 64289 Darmstadt, Germany — [3]Stem Cell and Developmental Biology, Technical University of Darmstadt, 64287 Darmstadt, Germany

Three-dimensional cellular models hold great promise for drug testing, but their success relies on maintaining a controlled supply of oxygen and nutrients. Artificial vascular networks aim to mimic blood vessel functions, yet ensuring robust endothelial cell (EC) attachment remains a significant challenge. In this study, we designed a mediator between artificial network surfaces and ECs using Poly(N-isopropylacrylamide) (PNIPAM) microgels (MGs) that remain mechanically stable in nutrient solutions. Charged MGs were synthesized and tested for adhesion on plasma-treated model surfaces. The microgel-coated substrates were exposed to cell static culture media and under defined flow. Atomic force microscopy (AFM) confirmed stable adhesion of MG particles before and after exposure. Initial experiments explored EC attachment on positively and negatively charged MG surfaces, followed by mechanical property characterization. The MG coatings were biofunctionalized with integrin-recognized ligands to enhance EC adhesion and proliferation further.

CPP 13: Molecular Electronics and Excited State Properties I

Time: Monday 17:15–18:30 Location: H38

CPP 13.1 Mon 17:15 H38

Revealing the Origin of low-energy Excited State Absorption in the nonlinear Optical Properties of Thiophene — •Mustapha Driouech, Michele Guerrini, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg

Optical nonlinearities in organic molecules are useful for advanced applications. Among them, optical limiting is particularly relevant to prevent critical damage to the human eyes and artificial sensors from intense radiation. In this ab initio study, we investigate the nonlinear optical properties of thiophene oligomers with a non-perturbative approach based on real-time time dependent density functional theory [1]. We study the optical absorption spectra obtained after applying a broadband instantaneous electric field. For sufficiently high intensities, we observe the appearance of absorption peaks at low energies that are not present in the linear spectra. To investigate in more details the nonlinear mechanisms involved, we perform pump-probe simulations combined with analysis of the population dynamics revealing that the emerging features are due to excited state absorption in the visible region. Our results show that this fully ab initio methodology is able to capture and unravel the fundamental mechanisms of optical nonlinearities in organic molecules.

[1] C. Cocchi, et al., Phys. Rev. Lett. 112, 198303 (2014).

CPP 13.2 Mon 17:30 H38

Theoretical perspectives on ground- and excited state absorption in organic materials: comparing TDDFT, GW/BSE, and post-Hartree-Fock methods — •Narges Taghizade[1], Andreas Windischbacher[1], Andreas W. Hauser[2], and Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]Institute of Experimental Physics, Graz University of Technology, Austria

Ground- and excited-state absorption (ESA) properties of conjugated organic materials are fundamental to the development of advanced optoelectronic devices. In this contribution, we specifically focus on molecules, which pose challenges to traditional theoretical approaches owing to significant electron correlation resulting in complex charge transfer and multi-reference characteristics, particularly when it comes to excited state properties. To address these complexities, we compute the ground and ESA spectra using a number of complementary, advanced theoretical methods. First, we employ time-dependent density functional theory within the linear and quadratic response frameworks, respectively. Second, we present results from a GW/BSE many-body perturbation theory approach thereby addressing the challenge of accurately accounting for charge transfer excitations. Third, we also apply post-Hartree-Fock methods, such as the multi-configurational self-consistent field method in order to tackle the strong electron correlation and multi-reference effects. The comparison of our results highlights the strengths and limitations of various computational approaches and offers a pathway toward improved theoretical models for the design of efficient optoelectronic materials.

CPP 13.3 Mon 17:45 H38

Charge and energy transfer mechanisms in a singlet fission donor-acceptor complex — •Karin S. Thalmann[1], Johan E. Runeson[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 is a photophysical process transforming a singlet excited electronic state to two triplet states [1]. Thus, materials exhibiting singlet fission have the potential to increase the efficiency of solar cells. Adding an acceptor to a singlet fission active molecule enables the extraction of charges and excitation energy. In our work, we study a diazadiborine dimer as donor [2] and tetracyanoquinodimethane as acceptor molecule. Using *ab initio* multireference perturbation theory calculations, we build a vibronic model Hamiltonian and further perform quantum dynamical [3] and mixed quantum-classical simulations [4] to analyse the charge and energy transfer dynamics in the complex. With our techniques, we characterise competing charge and energy transfer processes as well as intramolecular and intermolecular singlet fission. The analysis reveals the role of the different electronic states and vibrational modes in the dynamics of the donor-acceptor complex.

[1] M. B. Smith *et al.*, *Chem. Rev.* **110**, 6891-6936 (2010).
[2] T. Zeng, *J. Phys. Chem. Lett.* **7**, 4405-4412 (2016).
[3] S. R. Reddy *et al.*, *J. Phys. Chem. Lett.* **9**, 5979-5986 (2018).
[4] J. E. Runeson *et al.*, *J. Chem. Phys.* **159**, 094115 (2023).

CPP 13.4 Mon 18:00 H38

The Influence of Solvent Nature and Annealing Conditions on the TADF Properties of DMAC-TRZ in Films and Single Crystals — •Anatolii Kuimov[1], Sergey Bagnich[1], Christopher Greve[2], Eva M. Herzig[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth, Germany — [2]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Germany

We investigated the impact of molecular arrangement and post-processing conditions on the thermally activated delayed fluorescence (TADF) of the donor-acceptor type molecule DMAC-TRZ. Specifically, we studied luminescence at various temperatures and time delays after excitation across different solid-state morphologies, including amorphous films, polycrystals, and single crystals, complemented by X-ray analysis of the single crystal. In single crystals, we observed that emission energy, the singlet-triplet gap, and TADF intensity were influenced by processing conditions, such as aging, thermal and solvent annealing, and the choice of solution for crystal growth. These effects are attributed to changes in the torsion angle between the donor and acceptor moieties. Comparisons with polycrystals and amorphous films reveal that introducing morphological disorder promotes a more orthogonal donor-acceptor arrangement, leading to a smaller singlet-triplet gap and enhanced TADF. Our findings emphasize the pivotal role of molecular conformation in modulating photophysical properties. This study highlights the potential of tailoring material performance through structural modifications and annealing strategies to optimize TADF efficiency for organic optoelectronic applications.

CPP 13.5 Mon 18:15 H38

Effect of Junction Structure on Quantum Interference in Single-Molecule Junctions — •Aoshi Yamane, Shintaro Fujii, and Tomoaki Nishino — Department of Chemistry, School of Science, Institute of Science Tokyo, 2-12-1 Ookayama, Meguro-ku, Tokyo, Japan

The destructive quantum interference (DQI) effect in single-molecule junctions induces a steep decrease in electron transmission at specific energies, enables high on/off ratios of electrical conductivity, and is expected to be applied to molecular devices such as transistors and switches. Here, we aimed to elucidate the effects of molecular and molecule/metal interface structures on DQI. We focused on disubstituted naphthalene with different types and positions of anchoring groups connecting molecules and electrodes. Break junction measurements of the molecular junctions demonstrated that for naphthalenedithiol (NDT), 2,7-NDT showed significantly lower conductivity compared to 2,6-NDT, indicating the presence of DQI in 2,7-NDT. On the other hand, for naphthalenedicarbonitrile (NDCN), 2,6-NDCN and 2,7-NDCN showed similar conductance. Combined with Flicker noise analysis and DFT-NEGF transmission calculations, we demonstrate that the DQI features in 2,7-NDCN are masked by the contribution of electrode-π coupling, which short-circuit the molecular junctions. The present study provides important insights into the control of unique electron transport properties induced by DQI in single-molecule junctions.

CPP 14: Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)

Time: Monday 17:30–18:30 Location: H34

CPP 14.1 Mon 17:30 H34

Vapor-mediated wetting and imbibition control on micropatterned surfaces — •Ze Xu and Stefan Karpitschka — Fachbereich Physik, Universität Konstanz, Konstanz, Germany

Wetting and evaporation of droplets on micropatterned surfaces are ubiquitous in nature and key to many technological applications, such as water/ice-proof coatings, spray cooling, inkjet printing, and semiconductor surface processing. The wettability of micropatterned surfaces is governed by surface chemistry and topography, and significant effort has been devoted to overcoming this intrinsic behavior, e.g. to dry or coat structures surfaces, by use of external stimuli like electromagnetic fields. However, these methods usually require specific materials, thus limiting their practical use. Here, we show that the spreading behavior of water droplets on hydrophilic surface patterns can be controlled and even temporarily inhibited by the presence of the vapor of a low surface tension liquid. We show that this delayed wicking arises from Marangoni forces due to vapor condensation at the droplet periphery that compete with the capillary wicking force of the surface topography. We further demonstrate how modulating the vapor concentration in space and time can be used to guide droplets across patterns and even extract liquid from fully imbibed films, devising new strategies for coating, cleaning and drying of functional surface designs.

CPP 14.2 Mon 17:45 H34

Gradient dynamics model for volatile binary mixtures including Marangoni flows — •Jan Diekmann und Uwe Thiele — Universität Münster, Wilhelm-Klemm-Straße 9, 48149 Münster

We present a mesoscopic thin-film model in gradient dynamics form for binary liquid mixtures on solid substrates incorporating interface tension-induced flow, and volatility in a narrow gap. Thereby, we use and expand models established in [1-4] by accounting for the two substances in each of two bulk phases - liquid and gas - and for the enrichment of one component at the liquid-gas interface. We discuss the different contributions to the free energy, thereby employing Flory-Huggins theory of mixing for the condensed phase and assuming ideal gases for the vapor phase. The resulting five-field model is then analyzed with numerical time simulations focusing on the interplay of the drop dynamics with the developing lateral concentration gradients, and the resulting Marangoni flows. The results are compared to experimental findings [5].

[1] Thiele et al. Physical Review Fluids, 2016. doi: 10.1103/physrevfluids.1.083903.

[2] Xu et al. Journal of Physics: Condensed Matter, 2015. doi:10.1088/0953-8984/27/8/085005.

[3] Hartmann et al. Langmuir, 2024. doi: 10.1021/acs.langmuir.3c03313.

[4] Thiele et al. Physical Review Letters, 2013. doi: 10.1103/physrevlett.111.117801.

[5] Chao et al. Proceedings of the National Academy of Sciences, 2022. doi: 10.1073/pnas.2203510119.

CPP 14.3 Mon 18:00 H34

Fast dynamics of PNIPAM microgels at fluid interfaces: insights from droplet bouncing and jetting — Atieh Razavi, Suvendu Mandal, Benno Liebchen, Regine von Klitzing, and •Amin Rahimzadeh — Technische Universität Darmstadt, Hochschulstrasse 8, 64289 Darmstadt, Germany

PNIPAM microgels, as cross-linked polymer networks, are known to adsorb at the air-water interface, reducing surface tension. The kinetics of their adsorption, and thus the dynamic surface tension, depend on their cross-linking density, which determines the stiffness of individual microgels. Under interfacial perturbations such as dilation, softer microgels restore surface tension more rapidly, creating interfaces with higher surface elastic moduli, as shown by interfacial rheology studies using profile analysis tensiometry (1-10 s timescales). However, the behavior of microgels under very rapid interfacial deformations (milliseconds) remains unclear. We address this question through experiments involving droplet bouncing and jetting, processes relevant to applications such as inkjet printing and needle-free drug delivery. Our results demonstrate that microgels rapidly respond to fast interfacial deformations, with softer microgels restoring surface tension more efficiently. This quicker response allows greater interfacial extension in the presence of softer microgels. Molecular dynamics simulations corroborate our experimental findings, providing further insight into the mechanisms at play. This study highlights the critical role of microgel stiffness in determining their interfacial dynamics across a wide range of timescales and deformation rates.

CPP 14.4 Mon 18:15 H34

Soft dynamic wetting transition — •Christopher Henkel[1], Vincent Bertin[2], Jacco 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 and advancing dynamics of a three-phase contact line on a viscoelastic substrate, i.e., the wetting transition of a substrate from macroscopically dry to wet or vice versa. Thereby, we use the Landau-Levich (or dip-coating) geometry, where a solid viscoelastic plate is dragged out of or pushed into 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 changes with the plate velocity and the substrate softness. In this we compare numeric results with asymptotic analytic calculations. Finally, we explore whether the occurrence of stick-slip motion in the advancing case can be predicted, using simple scaling arguments.

CPP 15: Poster Session I

Time: Monday 19:00–21:00 Location: P4

CPP 15.1 Mon 19:00 P4

Exploring Green Solvent Additives for Enhanced Solubility in Organic Photovoltaics Processing — •Leonhard Schatt, Fabian Eller, and Eva M. Herzig — Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

Organic Photovoltaic (OPV) devices offer the potential for low-cost production of devices that convert light into electricity. These devices are typically processed from solution, which allows for simple, scalable production methods such as printing. However, the solvents used by most research groups are halogenated aromatic solvents, as green solvents often lack good solubility for the solutes used. We are therefore experimenting with additives in green solvents as a method of tuning solubility. We monitor the solubility with in-situ solubility measurements to study the effects of additive type and volume fraction. This will allow us to map the solubility space of the high performance OPV material PM6. Our aim is to contribute to the replacement of halogenated solvents for OPV processing and to make our organic electronic material processing feasible for industrial applications.

CPP 15.2 Mon 19:00 P4

Comparing Machine Learning Force Fields for Proton Transfer Dynamics in Solid Acids — •Jules Oumard, Aaron Flötotto, and Christian Dressler — Technische Universität Ilmenau, Fakultät für Mathematik und Naturwissenschaften, Institut für Physik, Fachgebiet Theoretische Festkörperphysik, Weimarer Straße 32, 98693, Ilmenau

Solid acids are excellent water-free proton conductors and can be used in fuel cells. [1]. The rarity of long-range proton transfer events in ab initio molecular dynamic simulations makes the calculation of converged diffusion coefficients challenging. This can be overcome by accelerating these simulations with machine learning force fields (MLFF). We compare two MLFF approaches: Gaussian Approximation Potentials (GAP) with on-the-fly learning [2] and equivariant graph neural networks [3]. A protocol for fine-tuning GAP models is presented. We evaluate the calculated diffusion coefficients and explain trends in terms of jump rate functions and anion rotation rates.

[1] Mohammad, N. et al. (2016). Journal of Power Sources, 322, 77-92. doi:10.1016/j.jpowsour.2016.05.021

[2] Jinnouchi, R. et al. (2019). Physical Review B, 100(1), 014105. doi:10.1103/PhysRevB.100.014105

[3] Batatia, I., et al. (2022). Advances in Neural Information Processing Systems. https://openreview.net/forum?id=YPpSngE-ZU

CPP 15.3 Mon 19:00 P4

Towards Theoretical UV/Vis Spectra with Experimental Accuracy. Benchmarks for Spiropyran Photoswitches — •Robert Strothmann[1], Johannes T. Margraf[2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Bayreuth

Molecular photoswitches are molecules that undergo an isomerization upon irradiation with specific wavelengths. One key feature for understanding this process are the UV/Vis spectra of the involved species (e.g. the closed and open forms in the case of spiropyran, SP). First-principles methods like density-functional theory (DFT) allow the calculation of UV/Vis spectra within certain approximations. However, the properties of the chosen functional, the description of solvation, as well as the accuracy of conformational and vibrational sampling all contribute to discrepancies between theory and experiment. This motivates us to establish a rigorous theoretical approach to assist in the prediction and analysis of UV/Vis spectra for molecular photoswitches. As a crucial step, we here benchmark different approaches for predicting UV/Vis spectra of SP switches against experimental references. We emphasize the influence of different functional approximations and highlight the role of the conformational ensemble and molecular vibrations sampling (e.g. via by machine learning enhanced molecular dynamics simulations). The importance of these different effects is discussed, with the goal of providing best practice guidelines that enable robust predictions.

CPP 15.4 Mon 19:00 P4

Optical properties of diamondoid organotin sulfur clusters with fluorescent ligands — •Alexander Schauerte[1], Jie Wang[2], Felix Thomas[1], Irán Rojas León[2], Stefanie Dehnen[2], and Marina Gerhard[1] — [1]Faculty of Physics and Material Sciences Center, Philipps-University of Marburg, Renthof 7a, D-35032 Marburg, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

White light is important in our daily life as well as in technology and research. It has been shown that diamondoid organotin clusters with organic ligands emit a brilliant white light beam when pumped with an infrared laser.

We investigate the fluorescent properties of tin-sulfur/selenium clusters with three phenyl- and one tetraphenylethylene ligands using photoluminescence- and spatially resolved photoluminescenceexcitation- spectroscopy. Through temperature-dependent measurements of compounds prepared as glass and as powder, we conclude that the electron-phonon-coupling and short-range ordering seems to be reduced in a glass state compared to a powder.

Furthermore, we investigate the white light generation (WLG) and second harmonic generation of different cluster compounds, which show a dependence of the WLG-efficiency on the chemical composition. The glass has a lower excitation power threshold for WLG than the powder.

CPP 15.5 Mon 19:00 P4

Electromagnetic Compatibility Measurements of Polymers in the Automotive Industry: Shielding Effectiveness According to ASTM D 4935 — Leopold Handke, Nicola Peranio, and •Verena Cerna — Technische Hochschule Ulm, Ulm, Deutschland

Electromagnetic compatibility (EMC) is a key concern in the automotive industry due to the growing complexity of vehicle electronic systems and the need to prevent electromagnetic interference that could affect their performance and safety. Polymers used in automotive components must meet specific EMC requirements to ensure proper functioning of vehicle electronics. This study investigates the shielding effectiveness (SE) of various polymer materials using standardized measurements according to ASTM D 4935. Shielding effectiveness for both magnetic (B-field) and electric (E-field) fields was measured over a frequency range from 50 kHz to 3 GHz. SE measurements provide valuable insights into the frequency-dependent shielding properties of plastics, offering a basis for selecting appropriate materials for automotive applications to address EMC challenges.

CPP 15.6 Mon 19:00 P4

Time-resolved structure formation in biohybrid coatings revealed by in-situ GISAXS and machine learning — •Julian E. Heger[1], Shachar Dan[2], Yufeng Zhai[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1] — [1]1TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [3]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden

Relationships between the structure and property of functional films are at the heart of material science, which makes understanding of how film morphology influences its function essential. Achieving a comprehensive and statistically relevant understanding of the film's characteristics often requires the use of indispensable tools like grazing-incidence small-angle X-ray scattering (GISAXS). GISAXS enables the exploration of the film's characteristic morphology in reciprocal space, such as characteristic size distributions. However, a challenge arises due to the loss of phase information during measurements, which inhibits a direct transformation from reciprocal space to real space via inverse Fourier transform. In addressing this obstacle neural networks (NN) emerge as promising solutions, as they offer potential ways to enable a fast transformation of GISAXS data. Here, we present the results of applying a NN which is trained on synthetic GISAXS data to evaluate the film formation of biohybrid coatings during deposition from in-situ GISAXS synchrotron data.

CPP 15.7 Mon 19:00 P4

Simulation-Based Neural Network with Embedded Prior

Knowledge for Predicting Morphological Parameters in GISAXS — •Shachar Dan[1], Eldar Almamedov[2], Matthias Schwartzkopf[1], Sven-Jannik Wöhnert[1], Andre Rothkirch[1], Yufeng Zhai[1], Jose I. Robledo[4], Volker Skwarek[2], and Stephan V. Roth[3] — [1]DESY, Notkestraße 85, D-22607 Hamburg — [2]HAW, Berliner Tor 5, D-20099 Hamburg — [3]KTH, Teknikringen 56 SE-10044 Stockholm — [4]FZ-Jülich, Wilhelm-Johnen- Straße D-52428 Jülich

In-situ grazing-incidence small-angle X-ray scattering (GISAXS) is a powerful technique for analyzing nanoscale structures, yet its interpretation is challenging due to the inverse problem caused by phase information loss. Advances in simulation software and deep learning techniques have opened the door to the idea of using simulations, which can now be generated more efficiently in diverse configurations, to train neural networks (NNs). However, simulations often fail to fully represent experimental data, creating a significant sim-to-real gap. In our work, we tackle this challenge by embedding prior knowledge about the system into the NN training process. By incorporating constraints based on this knowledge, we train models on simulations and apply them to experimental data, enabling reasonable predictions of morphological parameters such as cluster radii, inter-cluster distances, and grain size distributions. This approach aims to accelerate material characterization at the nanoscale and provide a portable and efficient counterpart to traditional methods.

CPP 15.8 Mon 19:00 P4

Low-Temperature Photoluminescence Characterization of Hybrid Metal Halides — •Anton Krüger[1], Meng Yang[2], Alexander Schauerte[1], Dominik Muth[1], Johanna Heine[2], and Marina Gerhard[1] — [1]Faculty of Physics and Material Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Faculty of Chemistry, Philipps-Universität Marburg, Hans-Meerwein-Straße 4, D-35032 Marburg, Germany

In order to remove the toxic lead component of the otherwise promising perovskite materials, many different approaches have been pursued.
Here, the photoluminescence (PL) and absorption properties of crystalline non-toxic hybrid main group metal halide compounds, (α-Me-2-NA)$_4$E$_2$X$_{10}$ (NA=Naphthylmethylammonium, E=Sb/Bi, X=Halide) are investigated by means of time-resolved PL spectroscopy, steady-state PL spectroscopy as well as PL excitation spectroscopy.
It is shown that the absorption and PL properties of these materials depend on the metal/halide composition, giving rise to a variety of absorbers and emitters. Furthermore, temperature dependent spectroscopic experiments reveal a thermochromic behavior of the compounds.

CPP 15.9 Mon 19:00 P4

Effect of fluorinated tail groups on the properties of aromatic self-assembled monolayers — Yangbiao Liu[1], Sonja Katzbach[2], Andreas Terfort[2], and •Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany. — [2]Institut für Anorganische und Analytische Chemie, Johann Wolfgang Goethe Universität Frankfurt, 60438 Frankfurt am Main, Germany

Electric transport properties of functional self-assembled monolayers (SAMs) are important for interface engineering in organic electronics and molecular electronics. As was shown recently, substituting only one terminal hydrogen atom in SAMs with a halogen atom changes their electric conductance noticeably. In this context, we studied the respective effects in a series of non-substituted and methyl-substituted biphenylthiolate (BPT) SAMs on Au(111), exchanging the terminal hydrogen atom/atoms for fluorine/fluorines and testing not only single-component but binary SAMs as well. The gradual variation of the work function with the SAM composition was accompanied by a gradual variation of electrical conductance, decreasing, in particular, by two orders of magnitude at going from CH3-BPT to CF3-BPT SAMs. The observed behavior was tentatively explained by the higher projected density-of-states at the position of the terminal tail groups in the CH3-BPT (H-BPT) case compared to CF3-BPT (F-BPT) and by the appearance of an internal electrostatic field in the SAMs, leading to a change and renormalization of the energy level alignments within the junction upon contact of the SAMs to the top EGaIn electrode.

CPP 15.10 Mon 19:00 P4

Charge separation in a porphyrin-based metal-organic framework incorporating fullerene — •Martin Richter[1], Xiaojing Liu[2], Pavel Kolesnichenko[1], Christof Wöll[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, Germany — [2]Institut für Funktionelle Grenzflächen, Karlsruher Institut für Technologie, Germany

Porphyrin-based materials are attracting great interest due to their wide range of potential applications. They can be embedded into metal-organic frameworks (MOF) to manipulate and investigate the relations between function and structure. In conjunction with an electron acceptor, charge separation can be achieved, which is beneficial for applications such as 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) with fullerene C$_{60}$ loaded into the pores, have demonstrated that photoexcitation can enhance 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 time scale. Charge separated states can be identified, which have a lifetime of 212-360 ps. The charge separation occurs after excitation of both the Soret band and the Q band within only a few hundred femtoseconds.

References

[1] X. Liu et al., Angew. Chem. Int. Ed. 2019, 58, 9590.

CPP 15.11 Mon 19:00 P4

Structural influences on nonlinear optical activity for supercontinum generation: isolated cubane — •Alexander Kapp and Simone Sanna — Institute for Theoretical Physics, 35392 Gießen, Germany

It has been suggested that adamantane-based molecular clusters can convert a narrowband laser source into a broadband supercontinuum. Unlike thermal emitters, the resulting spectra are coherent and not constrained by Planck's law, making them highly valuable for various applications, such as high-resolution monitoring and spectroscopy.

In order to expand our library of suitable molecules, we investigate the electronic and optical properties of materials with similar symmetry. This involves performing first-principle density functional theory calculations to identify appropriate structures. Here, we focus specifically on isolated cubane (C_8H_8) molecules and their derivatives, analyzing their electronic and structural properties and their correlation with the optical response.

CPP 15.12 Mon 19:00 P4

Impact of Classical and Quantum Light on Donor-Acceptor-Donor Molecules — •Haraprasad Mandal[1,2], Sajal Kumar Giri[3], Sara Jovanovski[1], Oleg Varnavski[1], Malgorzata Zagorska[4], Roman Ganczarczyk[4], Tse-Min Chiang[3], George C. Schatz[3], and Theodore Goodson III[1] — [1]Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109, United States — [2]Department of Chemistry, University of Graz, Heinrichstrasse 28, 8010 Graz, Austria — [3]Department of Chemistry, Northwestern University, Evanston, Illinois 60208, United States — [4]Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland

Investigations of entangled and classical two-photon absorption have been carried out for six donor (D)-acceptor (A)-donor (D) compounds containing the dithieno pyrrole (DTP) unit as donor and acceptors with systematically varied electronic properties. Comparing ETPA (quantum) and TPA (classical) results reveals that the ETPA cross section decreases with increasing TPA cross section for molecules with highly off-resonant excited states for single-photon excitation. Theory (TDDFT) results are in semiquantitative agreement with this anticorrelated behavior due to the dependence of the ETPA cross section but not TPA on the two-photon excited state lifetime. The largest cross section is found for a DTP derivative that has a single photon excitation energy closest to resonance with half the two-photon excitation energy. These results are important for the possible use of quantum light for low-intensity energy-conversion applications

CPP 15.13 Mon 19:00 P4

Correlating molecular properties to the SHG response: Prerequisites for white light generation. — •Ferdinand Ziese and Simone Sanna — Institut für Theoretische Physik and Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

Recent studies have demonstrated white light generation from molecular clusters with adamantane-like cores and different substituents [1,2]. Systematic investigations further our understanding of the origin of this behavior, we have investigated structural, electronic, and (nonlinear) optical properties from first principles for isolated molecules [3].

Core modifications mostly change the characteristic of the response in a more subtle manner while the exchange of substituents exhibit a greater impact. Distinct changes to the intensity, energy, and characteristic can be observed. The presented results provide a theoretical foundation for the design of tailored nonlinear optical sources.

[1] N. W. Rosemann, J. P. Eußner, A. Beyer, S. W. Koch, K. Volz, S. Dehnen, S. Chatterjee, Science 2016, 352, 1301

[2] N. W. Rosemann, J. P. Eußner, E. Dornsiepen, S. Chatterjee, S. Dehnen, J. Am. Chem. Soc. 2016 138 (50), 16224-16227

[3] Ziese, F., Wang, J., Rojas León, I., Dehnen, S., Sanna, S., 2024. J. Phys. Chem. A 128, 8360-8372

CPP 15.14 Mon 19:00 P4

Effect of Deposition Rates on the Morphology and Efficiency of Blue TADF OLEDs — •Tolga Durmus, Marius Schnapp, Ahmed Mohamed, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

The efficiency and stability of blue thermally activated delayed fluorescence (TADF) OLEDs are strongly influenced by the structural properties of their active layers. In this study, we investigate the impact of varying deposition rates on the morphology of these layers, focusing on their amorphous or crystalline nature. Atomic force microscopy (AFM) is used to analyze the surface morphology of the deposited layers and we aim to establish a correlation between the deposition conditions, the structural properties of the layers, and the efficiency of the OLEDs. These investigations are expected to provide valuable insights into optimizing fabrication parameters for improved blue TADF-OLEDs.

CPP 15.15 Mon 19:00 P4

Temperature-dependent Transient Electroluminescence of Blue TADF OLEDs — •Klara-Maria Bögle, Felix Kübert, Ahmed Mohamed, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

Third generation OLEDs use, in contrast to first and second generation OLEDs, ambient thermal energy to increase fluorescence, so-called Thermally-Activated Delayed Fluorescence (TADF). This is achieved via reverse inter-system crossing (*rISC*), which means that non-radiative triplet excitons are up-converted to radiative singlet excitons. This process significantly increases the internal quantum efficiency, up to 100%. In this study, OLEDs with the multiple resonance blue TADF emitter ν-DABNA embedded in an mCP matrix are investigated. Transient electroluminescence (EL) reveals a strong temperature dependence, which we model with rate equations to better understand the TADF process in an OLED under operating conditions. The rate equations describe the population densities of the triplets, singlets and charge carriers using the different rates of *(r)ISC*, triplet-triplet annihilation (*TTA*), triplet-polaron annihilation (*TPA*) as well as the (non-) radiative singlet/triplet decay rates. Traditionally, such analysis is often based on transient photoluminescence at room temperature, which also lacks charge carrier contributions and is thus inconclusive. We therefore aim to get a full picture of *all* population densities and recombination mechanisms to better understand efficiency limiting processes.

CPP 15.16 Mon 19:00 P4

Porous poly(ethylene glycol) films as a versatile platform for ssDNA immobilization and hybridization — Zhiyong Zhao and •Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

Poly(ethylene glycol) (PEG) films, fabricated by thermally induced crosslinking of amine and epoxy-terminated four-arm STAR-PEG precursors, were used as porous and bioinert matrix for single-stranded DNA (ssDNA) immobilization and hybridization. The immobilization relied on either the reaction between the amine groups in the PEG matrix and N-hydroxy succinimide (NHS) ester groups of the NHS-ester-decorated ssDNA or the reaction between the epoxy groups in the matrix and thiol groups of the respectively substituted ssDNA. The mixing ratio of the precursors was varied to tune the density of the amine and epoxy groups available for the immobilization. Spectroscopic and electrochemical data confirmed the successful immobilization of the ssDNA probes into the PEG matrix as well as the high hybridization efficiency, selectivity, and sensitivity of the resulting DNA sensors. Whereas these sensors were equivalent to the direct ssDNA assembly in terms of efficiency, they exhibited better selectivity and bioinert properties because of the bioinert character of the PEG matrix. The above findings place PEG films as a promising platform for highly selective ssDNA sensing, leveraging their flexible chemistry, 3D character, and bioinert properties.

CPP 15.17 Mon 19:00 P4

The effect of spherical nanoceria on the anionic polysaccharides and in vitro behavior as a wound dressing — •Alexandra Feraru[1,2], Zsejke-Réka Tóth[2], Klára Magyari[2,3], Monica Baia[4,5], Tamás Gyulavári[6], Emoke Páll[7], Emilia Licarete[8], Codrut Costinas[1,5], Oana Cadar[9], Ionel Papuc[7], and Lucian Baia[2,4,5] — [1]Doctoral School of Physics, Babes-Bolyai University, M. Kogălniceanu 1, 400084 Cluj-Napoca, Romania — [2]Nanostructured Materials and Bio-Nano-Interfaces Center, Interdisciplinary Research Institute on Bio-Nano-Sciences, Babes-Bolyai University, T. Laurian 42, 400271 Cluj-Napoca, Romania — [3]INSPIRE Research Platform, Babes Bolyai University, 400084, Cluj-Napoca, Romania — [4]Faculty of Physics, Babes-Bolyai University, M. Kogălniceanu 1, 400084 Cluj-Napoca, Romania — [5]Institute for Research-Development-Innovation in Applied Natural Sciences, Babes-Bolyai University, Fântânele 30, 400294, Cluj-Napoca, Romania — [6]Department of Applied and Environmental Chemistry, University of Szeged, Rerrich B. sqr. 1, Szeged 6720, Hungary — [7]Faculty of Veterinary Medicine, University of Agricultural Science and Veterinary Medicine, 400372 Cluj-Napoca, Romania — [8]Faculty of Biology and Geology, Babes-Bolyai University, 400015 Cluj-Napoca, Romania — [9]INCDO-INOE 2000, Research Institute for Analytical Instrumentation, 67 Donath Street, 400293 Cluj-Napoca, Romania

In this study, we aimed to enhance the understanding of how chemical bonds form when sodium alginate and gum arabic interact with nanoceria nanoparticles.

CPP 15.18 Mon 19:00 P4

Programming fibril alignment and mechanical response in electron beam-modified collagen type I fibers — •Friedrich Schütte[1,2], Anastassiya Bublikova[1,2], and Stefan G. Mayr[1,2] — [1]Division of Surface Physics, Department of Physics and Earth System Sciences, University of Leipzig, Linnéstr. 5, 04103 Leipzig — [2]Leibniz Institute of Surface Engineering (IOM), Permoserstr. 15, 04318 Leipzig, Germany

Modifying collagenous systems for tendon and tissue replacements in a controlled manner to produce biomimetic implants has a high potential for future biomedical applications. As a polymeric biomaterial, abundant in human bodies and influencing cellular morphology, collagen type I provides structural integrity and strength to tissues. However, applications are limited because even in crosslinked cases, the biomechanical properties of collagen networks can differ by several orders of magnitude in terms of both elasticity and load capacity. The widely used crosslinker glutaraldehyde has been the subject of controversy due to cytotoxic effects. In contrast, electron-beam-treatment allows reagent free control over a rapid and sterilizing crosslinking method in a non-cytotoxical biomimetic manner, resulting in improved mechanical properties due to high penetration depth and sufficiently high irradiation-induced doses. Subsequently, the modification of collagen type I fibers by energetic electron-beam-treatment during prestrain induced alignment of the inner filaments is shown to achieve and imprint network anisotropies resulting in mechanical properties with Young's moduli bridging orders of magnitude from a kPa range to a MPa range.

CPP 15.19 Mon 19:00 P4

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[1], Yusuf Bulut[1,2], Gergely Nemeth[3], Ferenc Borondics[3], Benedikt Sochor[1], Sarathlal K. Vayalil[1], Daniel Söderberg[4], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,4] — [1]Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [3]Synchrotron SOLEIL, Saint-Aubin, France — [4]KTH Royal Institute of Technology, Stockholm, Sweden

Cellulose has emerged as a promising bio-based template for 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 enhancements of the Raman signal over large areas. Herein, we present a straightforward approach utilizing the layer-by-layer spray coating method to fabricate films loaded with gold nanoparticles and graphene oxide to serve as SERS substrates. GISAXS combined with nano-FTIR spectroscopy was used to confirm a synergistic Raman enhancement mechanism of localized surface plasmon resonance and interface charge transfer. Our approach provides a reference for facile and scalable production of SERS substrates.

CPP 15.20 Mon 19:00 P4

Analysis of folding/unfolding behavior of micro and nano collagen fibers by SFTIRM — •Selcuk Kaan Haciosmanoglu[1], Gihan Kamel[2,3], and Murat Kazanci[1,4] — [1]Nanoscience and Nanoengineering Program, Graduate School, Istanbul Medeniyet University, Istanbul, Turkey — [2]SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East), Allan, Jordan — [3]Department of Physics, Faculty of Science, Helwan University, Cairo, Egypt — [4]Biomedical Engineering Department, School of Engineering and Natural Sciences, Istanbul Medeniyet University, Istanbul, Turkey

Collagen nanofibers are essential extracellular matrix (ECM) components widely used in regenerative medicine. While both electrospinning and wet-spinning techniques can produce anisotropic collagen micro- and nanofibers from dissolved collagen solutions, electrospun fibers require crosslinking to maintain water stability for cell culture applications. This study investigates in-situ crosslinking during electrospinning using chemical agents and physical methods. Synchrotron Fourier-Transform Infrared Microspectroscopy (sFTIRM) analysis revealed distinct molecular structural changes in the collagen nanofibers based on processing methods. Protein band positions shifted according to the extraction methods employed. Notably, electrospinning inhibited collagen molecule self-assembly, resulting in lower band positions compared to wet-spun fibers. The choice of crosslinking agent significantly influenced collagen's secondary structure, with genipin-mediated in-situ crosslinking better preserving the native structure of electrospun collagen nanofibers compared to UV crosslinking.

CPP 15.21 Mon 19:00 P4

Enhancing Endothelial Cell Attachment on PNIPAM-Based Microgel Coatings with RGD Ligand Functionalization — •Leonie Beer, Souraj Mandal, and Regine von Klitzing — Soft Matter at Interfaces, Department of Physics, Technical University of Darmstadt, Darmstadt 64289, Germany

Endothelial cell (EC) attachment is crucial for capillary formation and the success of artificial vascular networks in tissue engineering. Poly(N-isopropylacrylamide) (PNIPAM) microgels offer a promising platform for this application due to their tunable mechanical properties and ability to incorporate bioactive ligands. This study investigates the use of PNIPAM-based microgel coatings functionalized with the integrin-binding peptide sequence arginine-glycine-aspartate (RGD) to enhance EC adhesion. Successful conjugation of RGD peptides was confirmed using infrared spectroscopy and fluorescence microscopy. To evaluate the impact of ligand configuration, we compared three variations of RGD based peptides. The results reveal that increasing the anchor length significantly improves HUVEC recognition of the ligands, resulting in enhanced cell attachment and proliferation. These findings highlight the critical role of ligand design in optimizing biofunctional coatings. This work presents a straightforward chemical strategy for improving endothelial cell adhesion on PNIPAM-based microgel surfaces, paving the way for advanced artificial vascular networks in tissue engineering and regenerative medicine.

CPP 15.22 Mon 19:00 P4

Green plastics: Direct production from grocery wastes and characterization by using S-FTIR — •Onur Aras[1], Gihan Kamel[2,3], and Murat Kazanci[4,5] — [1]Istanbul Medeniyet University, Nanoscience and Nanoengineering Program, Graduate School, 34700 Istanbul, Turkey — [2]SESAME Synchrotron (Synchrotron-light for Experimental Science and Applications in the Middle East), 19252 Allan, Jordan — [3]Department of Physics, Faculty of Science, Helwan University, Cairo, Egypt — [4]Istanbul Medeniyet University, School of Engineering and Natural Sciences, Department of Biomedical Engineering, Istanbul, Turkey — [5]Istanbul Medeniyet University, Science and Advanced Technologies Research

This study investigates the production of cellulosic bioplastics from four green waste sources: hemp, parsley stem, pineapple leaves, and walnut shell, using either trifluoroacetic acid (TFA) or water as solvents. Synchrotron FTIR Microspectroscopy (SR-*FTIR) was employed to analyze structural modifications during biofilm formation and regeneration.Water-based biofilms retained their native cellulose, hemicellulose, and lignin components. In contrast, TFA-dissolved samples exhibited additional spectral bands in the hemicellulose region, attributed to ester bond hydrolysis and subsequent carboxylic acid formation. Principal component analysis revealed distinct groupings based on solvent type and polymer addition.

CPP 15.23 Mon 19:00 P4

How do stiffness patterns, with no topographical or chemical cues, influence cellular and tissue contact guidance? — •Mathis Grelier[1], Carlos Urena Martin[2], Mark Schvartzman[2], and Ana Suncana smith[1,3] — [1]Puls Group, Institute for Theoretical Physics and Interdisciplinary Center for Nanostructured Films (IZNF), Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany — [2]Department of Materials Engineering and Ilse Katz Institute for Nanoscale Science and Technology, Ben-Gurion University of the Negev, Beer-Sheva, Israel — [3]Group of Computational Life Sciences, Division of Physical Chemistry, Rudjer Bošković Institut, 10000 Zagreb, Croatia

While current systems cannot disentangle the effects of topography and stiffness contrasts, our study overcomes this challenge by investigating cell and tissue behavior on substrates with only alternating stiffness stripes. Our experiments and model reveal that wider stripes enhance alignment along stiffer or softer regions due to the higher energy cost of traversing softer substrates. At the cellular level, we employ a stochastic model based on Boltzmann weights applied to possible cell shapes, integrating energy contributions that govern movement across stiffness boundaries. For tissues, we extend this framework using a dissipative particle model to capture collective dynamics and mechanical interactions. To further explore these effects, we applied a Globalized Bounded Nelder-Mead optimization, enabling the efficient recovery of key physical parameters, such as stiffness and contractility, under both untreated and treated conditions.

CPP 15.24 Mon 19:00 P4

Latex film formation investigated by GISAXS and spectral reflectance — •Simon Schraad[1,2], Helder Marques Salvador[4], Nadja Kölpin[1], Nicolae Tomozeiu[4], Peter Müller-Buschbaum[2], and Stephan Volkher Roth[1,3] — [1]Deutsches Elektronen Synchrotron, Notkestraße 85, 22607 Hamburg — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [3]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Teknikringen 56, 100 44 Stockholm, Sweden — [4]Canon Production Printing Netherlands B.V., Van der Grintenstraat 10, 5914 HH Venlo, Niederlande

The film formation of latex inks on nanoporous substrates is of high interest for scientific and industrial applications. Inks are multicomponent, complex fluids and consist of colloids, pigments and solvents. The film formation is a multistage process. After deposition, solvent begins to evaporate and finally nanoparticles self assembly. To quantitatively analyze latex film formation a combination of in-situ grazing incidence small angle scattering (GISAXS) and light scattering will be employed. Here structural changes during the deformation and coalescence phase of latex colloids will result in changes in the scattering patterns. We present a design of an experimental spray chamber to allow in-situ GISAXS and the spectral reflectance during spray deposition of latex inks to be used at synchrotron facilities.

CPP 15.25 Mon 19:00 P4

Dynamic magnetic response of multicore particles: the role of grain magnetic anisotropy and intergrain interactions — •Ekaterina Novak[1], Elena Pyanzina[1], Andrey Kuznetsov[2], and Sofia Kantorovich[2] — [1]Ekaterinburg, Russia — [2]University of Vienna, Vienna, Austria

This study examines the magnetic properties of multicore magnetic nanoparticles (MMNPs) utilizing Brownian dynamics simulations in conjunction with the Landau-Lifshitz-Gilbert equation. We demonstrate that the magnetic responses of MMNPs, both static and dynamic, are governed by a complex interplay between the cores magnetic anisotropy and the strength of inter-core magnetic interactions. These insights are crucial for refining the design of multicore magnetic particles in various applications, including magnetic hyperthermia, data storage, and targeted drug delivery, where accurate control over magnetic characteristics is vital.

CPP 15.26 Mon 19:00 P4

Kinetics of nanostructure and interface evolution induced by photopolymerization — •Shouzheng Chen[1,2,3], Yufeng Zhai[2], Jungui Zhou[2], Guangjiu Pan[1], Sarathlal Koyiloth Vayalil[2], Rolf A.T.M. van Benthem[4], Johan F.G.A Janssen[5], Mats K. G. Johansson[6], Peter Müller-Buschbaum[1], and Stephan V. Roth[2,6] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]DESY, Notkestraße 85, 22607 Hamburg, Germany — [3]FRM II, Lichtenbergstraße 1, 85748 Garching, Germany — [4]Eindhoven University of Technology, Groene Loper 5, 5600, MB, Eindhoven, the Netherlands — [5]Covestro (Netherlands) B.V., Urmonderbaan 22, 6167, RD, Geleen, the Netherlands — [6]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Teknikringen 56, SE-100 44 Stockholm, Sweden

Photopolymerization offers spatial resolution, low energy consumption, and high curing speeds, making it a widely used technology in additive manufacturing. The kinetics of the physical transformation of the resin from liquid to solid (cross-linked) state induced by photopolymerization and the kinetics of the solid-liquid interface formation of resin multilayer are the key to achieving controllable high-precision manufacturing. By modulating precursor resin components and combining grazing incidence small angle X-ray scattering (GISAXS), the UV-curing induced nanostructure and the buried interface of resin multilayer are probed. We reveal how solvents and additive monomers determine in nanostructure and multilayer interface formation during photopolymerization.

CPP 15.27 Mon 19:00 P4

Effect of grafting density on particle distribution in polymer brush/gold nanoparticle composite materials — •Elias Hallenbach, Hayden Robertson, and Regine von Klitzing — Institute for Condensed Matter Physics, Technical University of Darmstadt, Germany

Metal/polymer nanocomposites are versatile hybrid materials and find use in many fields such as photonics, biomedical engineering and catalysis. A promising realization of this type of hybrid material is the controlled self-assembly of gold nanoparticles (AuNPs) inside a polymer brush, which induces color changes upon exposure to environmental changes enabling sensor applications.

The polymer brushes serve as a matrix for the immobilization of AuNPs. Particle uptake into the brush matrix is affected by parameters such as thickness, particle size and the grafting density. Polymer brushes with varying grafting densities are synthesized by a controlled polymerization (SI-ARGET ATRP) directly from a silicon substrate. The nanocomposite materials are fabricated by dip-coating of polymer brushes into a AuNP dispersion. Characterization of the nanocomposites is performed by (in situ) spectroscopic ellipsometry, atomic force microscopy and (in situ) X-ray reflectometry (XRR).

Uptake of nanoparticles has proven to be highest at intermediate grafting densities. I will discuss the influence of particle distribution inside the brush on particle uptake, which can be yielded by XRR measurements.

CPP 15.28 Mon 19:00 P4

Multi-material filament fabrication for 3D printing photo-electrocatalytic carbon nitride composites — •Timo Uhlein and Siowwoon Ng — FAU Erlangen-Nürnberg, Erlangen, Germany

Additive manufacturing of electrochemically active 3D structures is of rising interest. In particular, using fused deposition modeling (FDM) based on filament extrusion concept to produce carbon-polymer-based 3D structures offers several advantages, such as accessibility, low-cost and ease of use. Nevertheless, carbon-based filaments are limited with their applications. Therefore, incorporating additional materials to produce a multi-material filament is of interest, to create 3D-printed electrodes with new or targeted functional properties. In this project, we fabricated a multi-material filament consists of carbon nitride, C3N4, and carbon nanotubes, CNTs, for its photocatalytic properties and high conductivity, respectively, and polymer as the backbone of a FDM filament. We examined the performance of the composite C3N4-CNT electrodes for hydrogen evolution and the photocatalytic degradation of a dye. We indicate that further advancements can be achieved by developing multi-material filaments in order to use them for further electrochemical applications.

CPP 15.29 Mon 19:00 P4

Mechanochemical Behavior and Flow Dynamics of Glycerol Aqueous Solutions Confined between Ferrous Surfaces: Atomic-scale Insights from Reactive Molecular Dynamics Simulations — •Vahid Fadaei Naeini[1,2], Andreas Larsson[1], and Roland Larsson[2] — [1]Applied Physics, Division of Materials Science, Department of Engineering Sciences and Mathematics, Luleå University of Technology, Sweden. — [2]Machine Elements, Division of Machine Elements, Department of Engineering Sciences and Mathematics, Luleå University of Technology, Sweden.

This study explores the tribochemical behavior of glycerol and its aqueous solutions confined between ferrous surfaces using reactive non-equilibrium molecular dynamics simulations. Results show that glycerol reduces friction effectively, with viscosity decreasing as water content increases. Pure glycerol achieves lower friction but exhibits significant wall slip and deviations from a linear velocity profile near the surfaces. Glycerol dissociation, influenced by shear stress and pressure, produces water and organic acid by-products, with dissociation rates decreasing at higher water concentrations. Atomic-scale analysis reveals increased surface wear and iron atom dissociation under elevated stresses. These findings highlight the balance between friction reduction, viscosity, and tribochemical reactivity in glycerol-water mixtures, offering insights for sustainable lubricant design under extreme conditions.

CPP 15.30 Mon 19:00 P4

Evaluating the Properties of Nafion PEMFC Membrane via MD Simulations — •Mateja Jovanović[1], Matthias Baldofski[1], Igor Stanković[2], Marcin Rybicki[1], and Miljan Dašić[2] — [1]Freudenberg Technology Innovation SE & Co. KG, Hoehnerweg 2-4, 69469 Weinheim, Germany — [2]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia

Understanding the nanoscale interactions within Nafion membranes is crucial for optimizing their performance in Proton Exchange Membrane Fuel Cells (PEMFC). In present a molecular dynamics study of the structural and dynamic properties of Nafion-water systems under varying hydration levels using molecular dynamics simulations. The density of the Nafion-water system is examined to identify deviations from the ideal additivity rule, providing insights into molecular interactions and structural rearrangements. The radial pair distribution function, radius of gyration, pore-water contact surface, and diffusion coefficients for water and hydronium ions are analyzed to reveal the local organization, solvation quality, porosity, and transport properties within the hydrated Nafion membrane. The methodology used to obtain properties of the Nafion-water mixture builds on techniques previously developed for the study of ionic liquids [1].

[1] I. Stanković, M. Dašić, M. Jovanović, A. Martini, Langmuir 2024, 40(17), 9049-9058, doi:10.1021/acs.langmuir.4c00372

CPP 15.31 Mon 19:00 P4

Exploring Polymer Aging: Microscopy and Thermal Analysis — •Judith Bünte, Laila Bondzio, Karsten Rott, and Andreas Hütten — Universität Bielefeld, Dünne Schichten und Physik der Nanostrukturen, Universitätsstr. 25, 33615 Bielefeld

The analysis of polymers and their additives is essential for understanding material performance and longevity, particularly in the context of aging processes. This work emphasizes the synergistic application of advanced microscopy and thermal analysis techniques to investigate polymer composition, structure, and degradation behavior.

Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy (SEM) were utilized to visualize the microstructural features of polymer matrices, as well as the distribution of particles within the polymer. TEM offered high-resolution imaging to reveal morphological details, while SEM enabled surface characterization. These imaging techniques were further augmented by Differential Scanning Calorimetry to analyze thermal properties.

Polymer aging was studied under controlled conditions to evaluate structural and compositional degradation over time. Changes in microstructure and thermal properties were correlated with aging-related alterations.

The integration of these analytical techniques establishes a robust framework for characterizing polymers and their additives. This approach yields valuable insights into the stabilizing role of additives, such as TiO_2, in protecting polymers against environmental and thermal stressors.

CPP 15.32 Mon 19:00 P4

Atomistic simulations of PEDOT:PSS — •Richard Schömig[1,2], Annalena Riffelt[2], and Alexander Schlaich[1] — [1]Institute for Atomistic Modeling of Materials in Aqueous Media, Hamburg University of Technology, Hamburg — [2]SC SimTech, University of Stuttgart, Stuttgart

PEDOT:PSS is by far the best known conjugated polymer with a broad application in e.g. bioelectronics, energy storing devices or neuromorphic computing due to its electrolyte-dependent swelling behavior and extraordinary conductance in the doped (oxidized) state. However, the insolubility of its films once their dried hinders classic experimental studies, thus making molecular dynamics simulations an indispensable tool to understand its electronic and mechanical behavior on an atomic scale. Here, we employ different established force fields to study the influence of a set of parameters such as different water models, dissociation degrees, partial charges and simulation protocols on the structural changes and polymer physics by water uptake for both the PEDOT and the PSS part. We test the validity of these force fields by benchmarking them against ab-initio MD and experimental results.

CPP 15.33 Mon 19:00 P4

Analysis of the Reciprocity Theorem in the DWBA — •Reinhard Sigel — Independent Scientist, D-88677 Markdorf, Germany

The Distorted Wave Born Approximation (DWBA) is a favored theory among X-ray scientists for the analysis of interface scattering experiments [1,2]. Unfortunately, there is no proper clarification which X-ray specific aspects and approximations enter the DWBA and what is the difference to interface scattering of coherent visible laser light. Based on the differing refractive index approaches for X-rays and for visible light, we identify the spot where an X-ray specific equation enters the derivation [1] of the so-called reciprocity theorem. It involves an intermixing of microscopic and macroscopic Maxwell equations. A much simpler correct derivation valid for both wavelength ranges is discussed.
[1] Daillant, Gibaud, *X-ray and Neutron Reflectivity*, Springer 2009.
[2] Renaud, Lazzari, Leroy, Surf. Sci. Reports 64, 255–380 (2009).

CPP 15.34 Mon 19:00 P4

Dynamic Polarization and Electrostriction of PVDF-Based Copolymer Films as Measured with Double-Modulated Interferometry — Marvin Malchau[1], Philipp Ramming[2], and •Lothar Kador[1] — [1]University of Bayreuth, Institute of Physics and BIMF, 95440 Bayreuth, Germany — [2]University of Bayreuth, Experimental Physics II, 95440 Bayreuth, Germany

Thin films of a ferroelectric copolymer based on polyvinylidene fluoride (PVDF) were exposed to electric ac fields with amplitudes up to 115 MV/m and frequencies between 5 and 100 Hz. The electrical polarization of the material was calculated by integrating the current flow, and the electric-field-induced thickness change (electrostriction) was measured with double-modulated interferometry. Thickness changes up to 60 nm were observed in an 8 μm thick film. The polarization shows a hysteresis loop typical for ferroelectric materials; it is independent of frequency in the investigated frequency range. The electrostriction exhibits a different type of hysteresis with strong frequency dependence. This indicates that the mechanical relaxation of the polymer film is independent of the electric dipole orientation.

CPP 15.35 Mon 19:00 P4

Ternary Organic Solar Cells For Space Applications — •Ivonne A. Zitzmann, Lukas V. Spanier, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

It has been demonstrated that organic solar cells (OSC) are capable of achieving high gravimetric power density, making them suitable for space applications. However, they still exhibit insufficient long-term stability, and there are few studies on their performance under space-like conditions. Here we investigate the ternary OSC system PBDB-T-2F:BTP-eC9:PC$_{71}$BM by optimizing its efficiency and studying its structure and degradation by optical measurements and grazing incidence wide and small angle X-ray scattering. Space conditions were simulated with AM0 illumination. Further, the OSCs were exposed to temperature cycling to assess their stability in a space environment, subject to rapidly changing temperatures. In addition, data from a suborbital rocket flight was examined for performance and degradation of the solar cells. These results may allow for the furthering of our understanding of photovoltaic power generation in harsh environments.

CPP 15.36 Mon 19:00 P4

Degradation of Printed Organic Solar Cells at High Temperatures — •Christoph G. Lindenmeir[1], Simon A. Wegener[1], Christopher R. Everett[1], Julian E. Heger[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Elettra, 34149 Basovizza, Trieste, Italy

Organic solar cells (OSCs) have gained significant attention recently due to their non-toxicity, short energy payback times, and fast efficiency improvements. Their high absorbance, potentially flexible design, and easy solution-based manufacturing make them particularly promising. Especially slot-die printing, a fast and low-waste fabrication method, enhances their scalability and potential for various applications, including space use. OSCs are particularly suited for space as their thin, lightweight structure provides a higher power-to-weight ratio than traditionally used solar cells, lowering production and launch costs. However, space conditions like extreme temperatures, high vacuum, and radiation accelerate degradation. This study focuses on the impact of extreme temperature variations on printed OSCs. We optimized their printing process and analyzed their degradation using operando grazing incidence small-angle X-ray scattering (GISAXS), a nondestructive method for studying thin-film morphology. Additionally, we monitored their electrical performance under high vacuum to simulate space conditions.

CPP 15.37 Mon 19:00 P4

Modulate Pre-aggregation to Optimize the Morphology in Organic Solar Cells — •Tim Bohnen, Jinsheng Zhang, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Morphology optimization has emerged as a key strategy to effectively improve device performance and stability in organic solar cells. Due to the solution-processing method, the selection of solvents for precursor solutions is crucial, as it directly affects the ultimate the morphology of active layer. Recent research demonstrates that donor and acceptor molecules form aggregates of varying sizes in precursor solutions, subsequently inducing different phase separation and crystallization behavior during drying process. However, the detailed correlation between pre-aggregation behavior and final morphology has yet to be fully elucidated. In this study, the active layer is composed of PBDB-TF-TTz acting as the donor and BTP-4F-24 as the non-fullerene acceptor. Next, we characterize the resulting morphology using atomic force microscopy (AFM) and grazing incidence small- and wide-angle X-ray scattering (GIWAXS and GISAXS).

CPP 15.38 Mon 19:00 P4

Investigation of quenching in exciplex OLEDs under variation of the giant surface potential — •Clarisse Henriques, Albin Cakaj, Alexander Hofmann, and Wolfgang Brütting — Institut für Physik, University of Augsburg, Augsburg, Germany

An exciplex is a short-lived excited charge transfer state formed between donor and acceptor molecules of different species, in which under radiative decay a photon is emitted. They can either function as efficient host for emitters or directly as emitter because of their apparent thermally activated delayed fluorescence characteristics. Especially the electron accepting materials tend to show a macroscopic film polarization, which is also referred to as giant surface potential (GSP). The presence of GSP in an organic light emitting diode (OLED) promotes charge injection in the electron transport layer (ETL), but causes the accumulation of holes, which can result in exciton quenching. Consequently, studying the impact on the device is of crucial importance. The main interest lies now on the tunability of this parameter by using the material as a co-host or directly as emitter. We investigate OLEDs with different film thickness of the ETL and emission layer. Additionally, devices of donor and acceptor with different mixing ratios were prepared. The major focus is now on studying these systems by current density-voltage-luminance, photoluminescence (PL) and electroluminescence spectra, impedance spectroscopy and their PL quenching under different bias voltages. Such studies are fundamental to understand the impact of SOP in OLEDs for further improvement.

CPP 15.39 Mon 19:00 P4

Tracking degradation of non-fullerene organic solar cells under dynamic environmental conditions — •Lixing Li, Lukas Spanier, Zhaonan Jin, Linus Huber, Guangjiu Pan, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

The power conversion efficiency (PCE) of non-fullerene organic solar cells (OSCs) has already approached 20%, but stability and environmental degradation issues have always been one of the biggest challenges limiting their application. Considerable research has been conducted to understand the degradation mechanisms in OSCs, especially under extreme environmental conditions like high and low temperatures. While these studies offer valuable insights, they do not fully represent the dynamic conditions that most organic solar cells face in real-world environments. In practical scenarios, environmental factors such as temperature, humidity, and light fluctuate over time rather than remaining constant. Therefore, it is crucial to investigate how OSCs degrade not only under steady stress but also when exposed to varying environmental conditions. This study explores the degradation of BTP-4F non-fullerene organic solar cells subjected to multiple environmental cycles. Advanced characterization methods, including grazing-incidence X-ray scattering (GIXS) and atomic force microscopy (AFM), are used to monitor both in-situ and ex-situ structural changes in the active layer of OSCs, offering deeper insights into the underlying degradation mechanisms.

CPP 15.40 Mon 19:00 P4

Revealing the Effect of Solvent Vapor Annealing on the Morphology of Non-Fullerene Organic Solar Cells — •Liansong Chu — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Solvent vapor annealing (SVA), as an effective post-treatment technique, has been widely used to optimize the morphology in organic solar cells (OSCs). When exposed to the specific solvent atmosphere, the swelling effect induced by solvent vapor facilitates molecular mobility of both donor and acceptor molecules, leading to modifications in crystallinity and phase separation. Hence, the selection of solvent and annealing duration for SVA is critical for the morphology, which ultimately determines the power conversion efficiency and stability. However, fundamental understanding of solvent selection criteria and the associated kinetic processes during treatment remains unknown. In this work, we systemically investigates the impact of different solvents for SVA on the morphological properties of non-fullerene OSCs (PBDB-TF-TTz as the donor and BTP-4F-24 as the acceptor) using atomic force microscopy (AFM), grazing incidence small- and wide-angle X-ray scattering (GISAXS and GIWAXS). Furthermore, we provide real-time insights into the morphological evolution during SVA through in situ UV-Vis absorption spectroscopy and photoluminescence measurements.

CPP 15.41 Mon 19:00 P4

Impact of the electrode area on the local J-V curves of organic photovoltaics — •Paul Schwanitz[1], Fabian Eller[1], Carsten Deibel[2], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Organic photovoltaics (OPV) are promising candidates for flexible solar cells, which may be more cost efficient to produce than their silicon counterparts. The organic semiconductor materials can be dissolved and printed on large scale, with the attractive advantage that the geometry of the OPV devices can be chosen on demand. The aim here is to analyze the influence of the top and bottom size of the electrodes on the J-V curve measurements. If the active areas are too small, fluctuations in the performance can occur, which are caused by inhomogeneities in the film. As the active area increases, performance is expected to stabilize as it is averaged over a larger area [1]. The different sizes of the anode and cathode also enable in-line measurements during production. The sizes of the electrodes are systematically varied to estimate the influence on the measurements, to interpret the J-V curves correctly and to account for the dark currents.

[1] Herzig, E. M., Gao, F., Bergqvist, J., Loi, M. A., & Meier, S. B. Harmonizing organic photovoltaics research and development among academia and industry. Joule, 8, 2171 (2024). https://doi.org/10.1016/j.joule.2024.07.015

CPP 15.42 Mon 19:00 P4

Thin Films of Substituted Benzo[*b*]fluorenes as Emitting Layers for Blue OLED Devices — •Pascal Schweitzer[1], Christopher M. Leonhardt[2], Cazibe Arslan[1], Hermann A. Wegner[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen — [2]Justus-Liebig-Universität Gießen, Institut für Organische Chemie, Heinrich-Buff-Ring 17, D-35392 Gießen

Organic light emitting diodes (OLED), despite widespread application in displays, still exhibit major challenges: The search for stable and efficient blue-emitting molecules continues, as these often suffer from degradation. Here we study substituted benzo[*b*]fluorenes (BF) as an alternative for such emitters. Their modular structure allows for tuning opto-electronic properties. Thin films of different BF were prepared by solution-based methods or physical vapor deposition (PVD). Significant blue emission was found by photoluminescence spectroscopy in solid state. Film growth at device interfaces was studied. In-situ Kelvin-probe force microscopy (KPFM) gave insight into electrical contact formation to typical transport materials: Stranski-Krastanov growth was found in PVD onto hole-conducting poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), accompanied by the formation of an interface dipole. On the electron-conducting side, a pronounced Volmer-Weber growth of bathocuproine (BCP) on the emissive layer demands a high film thickness for pinhole-free contacts. Finally, based on these findings, we show a working prototype of a blue OLED based on a substituted BF.

CPP 15.43 Mon 19:00 P4

Excimer as intermediate in singlet fission process for Polydiketopyrrollopyrole based materials — •Sruthy Asa Rajan, Sergey Bagnich, and Anna Köhler — University of Bayreuth, Bayreuth, Germany

Photovoltaics are essential for renewable energy generation, but the efficiency of conventional solar cells is constrained by the Shockley-Queisser limit, which arises from fundamental and practical losses such as thermalisation loss. Singlet fission (SF), a carrier multiplication process, offers a promising pathway to surpass this efficiency limit. However, a key challenge lies in identifying SF molecules with triplet energy levels that align with the silicon band gap, enabling the efficient formation of correlated triplet pairs, 1(TT) and their subsequent separation into individual triplets.

Polydiketopyrrollopyrole (PDPP) is a molecule with a comparable triplet energy to the silicon bandgap. We investigate the influence of solvent properties on the optical behaviour of N-substituted pyrene-bridged PDPPs. We employ temperature-dependent steady-state and time-resolved photoluminescence studies on N-substituted pyrene-bridged PDPPs in protic polar and aprotic polar solvents to study the evolution of different species. We observe excimer emission at intermediate temperature and 1(TT) emission at lower temperature. This observation supports the notion that excimers are involved in the formation of 1(TT).

CPP 15.44 Mon 19:00 P4

Solution processed organic solar cells for agrivoltaic applications — •Sebastian Coen, Yunan Chen, Kerstin Märkle, and Christian Sprau — Karlsruhe Institute of Technology, Light Technology Institute

Organic solar cells (OSCs) offer a wide range of applications due to their light weight, low energy payback time, non-toxicity and mechanical flexibility. This work aims to expand these applications by fabricating semitransparent OSCs for agricultural photovoltaic applications, such as greenhouses and foil tunnels.

To facilitate future industrial production, we explore scalable processes and a fully solution-processed architecture based on non-halogenated solvents. The fabricated solar cells are studied in terms of their electrical and spectral properties and their real space morphology.

CPP 15.45 Mon 19:00 P4

Utilizing Ultrasonic Spray for the Integration of Organic Solar Cells on Cellulose Substrate — •Xinyu Jiang[1], Kang An[2], Qin Wang[2], Nadja Koelpin[1], Arik Willner[1], Ning Li[2], and Stephan V. Roth[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg — [2]Institute of PolymerOptoelectronic Materials and Devices, State Key Laboratory of Luminescent Materials and Devices, South China University of Technology (SCUT), Guangzhou, Guangdong 510641, China — [3]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Teknikringen 56-58, SE-100 44 Stockholm, Sweden

Cellulose nanofibrils, heralded for their eco-friendly and renewable nature, offer a significant stride toward sustainable energy solutions. Their advantageous attributes such as biocompatibility, flexibility, lightweight nature, transparency, and remarkable mechanical strength render them suitable as a base material for incorporating photovoltaic or electronic devices. We aim to explore the development of functional photovoltaics on transparent cellulose-fabricated curtains, aiming at transforming undesired sunlight into electricity. The inherent flexibility of curtains poses a fabrication challenge for solar cells, adeptly mitigated through ultrasonic spray deposition. This technique manifests as an efficacious means to engender functional layers on a large scale, ensuring a homogeneous surface with minimal roughness. Employing an advanced non-fullerene acceptor system, the resultant organic solar cell curtain showcases the promising performance, delineating a path toward substantial applications in the sustainable energy.

CPP 15.46 Mon 19:00 P4

Multiscale morphological modulation in spray-coated organic solar cells — •Shuxian Xiong[1,2], Benedikt Sochor[1], Constantin Harder[1,2], Sarathlal Koyiloth Vayalil[1], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,3] — [1]Deutsches Elektronen-Synchrotron 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

The balance between phase separation and crystallization arising from the aggregations of organic semiconductor molecules defines the film morphology, resulting in multi-length scale phase transitions that enhance device performance. We investigate the morphological evolution driven by molecular self-assembly during the ultrasonic spray-coating of organic functional layers in organic solar cells. An in-depth understanding of phase transition phenomena through an analysis of both temporal (film formation kinetics) and thermal scales (annealing), with the elucidation of the intricate structure-performance nexus linked to morphological evolution and device efficiency, is achieved. We clarify the principles of effective morphological optimization to achieve high-efficiency sprayed organic solar cells, providing valuable guidance for their commercial application.

CPP 15.47 Mon 19:00 P4

Impact of amphiphilic additives on organic solar cells: Enhancing thermal stability for long term performance — •Jose Prince Madalaimuthu[1,2], Tim Matzdorff[1,2], Zhuo Xu[1,2], Md. Moidul Islam[1,2], Yisak Tsegezab Gerase[3], Hassan Ismail[1,2], Rico Meitzner[4], Aman Anand[1,2], Martin Presselt[3], Ulrich S Schubert[1,2], and Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-University Jena, Jena, Germany — [2]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller- University Jena, Jena, Germany — [3]Leibniz Institute of Photonic Technology (IPHT), Jena, Germany — [4]Helmholtz-Zentrum Berlin GmbH, Hahn-Meitner Platz 1, 14109 Berlin, Germany

The stability of organic solar cells (OSCs) depends not only on the device architecture or effective sealing but also significantly on the morphological stability of the photoactive layer. This stability can be disrupted by alterations in the spatial arrangement of the electron donor and acceptor, which are the fundamental components of OSCs. The extent of phase separation between donor and acceptor regions within the bulk heterojunction (BHJ) plays a pivotal role in determining device performance. Consequently, various strategies have been explored to preserve the distribution of these components. One promising approach is the incorporation of amphiphilic molecules to enhance the stability of the donor-acceptor interface. This method improves thermal resilience, overall OSC performance, and mitigates morphological degradation.

CPP 15.48 Mon 19:00 P4

Interfacial encapsulation of organic solar cells — •Saib Jahan Qazi[1,2], Md Moidul Islam[1,2], Zhou Xu[1,2], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich Schiller- University Jena, Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-University Jena, Jena, Germany

Organic solar cells are emerging as promising prospects in the field of solar energy technology due to their low-cost, light-weight and simple roll to roll fabrication properties. A record power conversion efficiency above 19% has already been reported. However, long-term stability is still the main obstacle for commercialization of these devices. In this study, we demonstrate solution processed interlayer encapsulation of organic solar cells using polymer-based barriers to prevent interlayer migration of impurities as well as the ingress of oxygen and moisture.

CPP 15.49 Mon 19:00 P4

Modifying spacers for higher efficiency and stability of single-component organic solar cells — •Yakun He[1], Peter Baeuerle[2], Weiwei Li[3], Christoph Brabec[4], and Frederic Laquai[1,5] — [1]King Abdullah University of Science and Technology, Saudi Arabia — [2]University of Ulm, Germany — [3]Beijing University of Chemical Technology, China — [4]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [5]Ludwig-Maximilians-Universität München, Munich, Germany.

Organic solar cells have achieved 20% efficiencies yet still lag regarding stability. Single-component materials incorporating donor and acceptor moieties in a nonconjugated method exhibit intrinsically high stability because of the restriction of morphological evolution. Nevertheless, the efficiency of single-component organic solar cells (SCOSCs) is still low compared to bulk heterojunction structures. We employ a series of dyads with similar structures but modify their spacer type and lengths to investigate the structure-morphology-performance relation. Photophysics has been studied by using steady-state and transient absorption and photoluminescence. Dyad4, with a proper long spacer, has shown the highest efficiency and surprisingly high stability under illumination. Moreover, we investigated the thermal stability of double-cable polymers by tuning the linker length between donor and acceptor moieties. Surprisingly, double-cable polymers do not show a decline of stability with the increase of space linker, and all of them display remarkably excellent stability without degradation after heating for 1000 hours at 90 degree.

CPP 15.50 Mon 19:00 P4

Photoinduced charge transfer and photophysics of functionalized Diethienopyrrole molecules from first principles — •Jannik Theile, Caterina Cocchi, and Michele Guerrini — Physics Department and Center for Nanoscale Dynamics, Carl von Ossietzky Universität Oldenburg, D-26129 Oldenburg, Germany

Donor-acceptor compounds are key components in organic electronics due to their tunable electronic and optical properties. In this work based on time-dependent density functional theory, we examine diethienopyrrole molecules, which act as electron donors, covalently combined with electron-acceptor units, focusing on their charge transfer dynamics induced by femtosecond laser excitations.
In the current symmetric molecule configuration, we find strong fluctuation patterns of the charge after laser excitation across both intensities and with and without nuclear motion, exceeding the initial changes of charge induced by laser excitation and the charge transfer (CT) remains insufficient and inconsistent throughout time evolution. Further considerations include asymmetric molecule configuration.

CPP 15.51 Mon 19:00 P4

Direct stochastic optical reconstruction microscopy (dSTORM) on cationic copolymer microgels — •Evelyn Gettinger and Thomas Hellweg — Physical & Biophysical Chemistry, University Bielefeld, Bielefeld, Germany

Microgels, three-dimensional polymer networks with colloidal dimensions, are promising candidates for catalysis, sensory and drug delivery applications due to their responsive properties. Cationic copolymer microgels, in particular, are gaining increasing attention in research, as they are suitable for conjugation with biomolecules like peptides, antibodies, and nucleic acids. Poly(NNPAM-co-DAPMA) is one such microgel that exhibits thermoresponsiveness through the monomer N-n-propylacrylamide (NNPAM) and pH responsiveness through the cationic comonomer N-3-(dimethylamino)propylmethacrylamide (DAPMA). This study investigates the network structure of Poly(NNPAM-co-DAPMA) microgels using direct stochastic optical reconstruction microscopy (dSTORM), a high-resolution fluorescence technique. Microgels with varying DAPMA concentrations were synthesized and analyzed for swelling behavior and polydispersity using photon correlation spectroscopy (PCS). Morphological properties were examined with atomic force microscopy (AFM). Post-synthetic fluorescence labeling with the anionic dye DY-654-carboxylic acid revealed a gradient of fluorophore localization from the core to the periphery and concentrated fluorophore domains, indicating a heterogeneous network with random comonomer distribution.

CPP 15.52 Mon 19:00 P4

Volume phase transition of NIPAM based copolymer microgels with non-thermoresponsive comonomers — •Jannis Krüger and Thomas Hellweg — Physical and Biophysical Chemistry, Bielefeld University

We conducted photon correlation spectroscopy (PCS) to obtain swelling curves of *N*-isopropylacrylamide (NIPAM)-based copolymer-microgels with varying content of non-thermoresponsive *N*-tert-butylacrylamide (NtBAM). Increasing NtBAM content reduces the hydrodynamic radius and broadens the volume phase transition (VPT). We analyzed the thermoresponsive contribution to the swelling curves with a cooperative Hill-like model for the Flory-Huggins interaction parameter $\chi_{\text{Hill}}(T)$ [1]. This model effectively describes the microgel swelling at various compositions. The Hill parameter ν estimates the number of water molecules leaving a polymer segment at the phase transition. A linear decrease of ν with BIS content suggests that water stays adsorbed on BIS during the VPT due to the lack of an LCST [2]. We fitted PNIPAM-*co*-NtBAM microgel swelling curves [3] with a hybrid model of χ_{Hill} for NIPAM and the original Flory-Huggins parameter χ_{FH} for NtBAM, revealing an exponential decrease in ν with x_{NtBAM}, indicating that NtBAM inhibits water adsorption of neighboring NIPAM units. Based on these results we propose a steric mechanism, which qualitatively describes the observed inhibition of microgel hydration.
[1] D. C. Leite et al., Langmuir 34 (2018), 10943. [2] S. Friesen et al., Gels 7 (2021), 42. [3] J. Krüger et al., Colloid Polym. Sci. (2024).

CPP 15.53 Mon 19:00 P4

Amphiphilic Monomers Bridge Hydrophobic Polymers and Water — •Guido Kusters[1,2,3], Guogao Zhang[1,4], Zheqi Chen[1,5], and Zhigang Suo[1] — [1]Harvard University — [2]Eindhoven University of Technology — [3]Max Planck Institute for Dynamics and Self-Organization — [4]Xi'an Jiaotong University — [5]Zhejiang University

Water dissolves a hydrophilic polymer but not a hydrophobic polymer. However, many hydrophilic polymer monomers are amphiphilic, with a hydrophobic vinyl group for radical polymerization and a hydrophilic group, and so may form solutions with both water and hydrophobic polymers. Ternary mixtures of amphiphilic monomers, hydrophobic polymers, and water have recently been used as precursors for interpenetrating polymer networks with unusual properties. However, the phase behavior of such ternary mixtures has not been studied. Here we mix the amphiphilic monomer acrylic acid, the hydrophobic polymer poly(methyl methacrylate) and water. In the mixture, the hydrophobic polymer can form various morphologies, including solution, micelle, gel, and polymer glass. We interpret these findings by proposing that the hydrophobic and hydrophilic groups of the amphiphilic monomer enable it to function as a bridge. That is, the hydrophobic functional group binds to the hydrophobic polymer, and the hydrophilic functional group binds to water. This picture leads to a simple modification to the Flory-Huggins theory, which agrees well with our experimental data. Amphiphilic monomers offer a rich area for the development of materials of self-assembled structures with unusual properties.

CPP 15.54 Mon 19:00 P4

Mechanical Characterization of Epon 862/DETDA Epoxy Networks: Molecular Dynamics Simulations — •Djihed Rezzig[1,3], Wolfgang Verestek[2], Saad Abdeslam[1], Johannes Roth[3], and Siegfried Schmauder[2] — [1]LPMMM, Setif 1 University-Ferhat ABBAS, Algeria — [2]IMWF, Stuttgart University, Germany — [3]FMQ, Stuttgart University, Germany

Epoxy resins are widely used in advanced materials due to their exceptional mechanical properties. Among them, Epon 862/DETDA is a commonly employed thermoset system in aerospace and automotive applications. This study employs molecular dynamics simulations to investigate the mechanical behavior of the Epon 862/DETDA epoxy network. The simulations were conducted using cross-linked molecular models to represent the cured network, incorporating detailed atomic scale interactions. Mechanical behavior was evaluated by simulating stress-strain responses under tensile loading conditions and shear test for the elasticity tensor, revealing the epoxy networks high modulus and strength. Additionally, the study examines the effects of varying cross-link densities and molecular configurations on the materials performance.

CPP 15.55 Mon 19:00 P4

The effect of intracrystalline chain dynamics (ICD) in the stress relaxation of semi-crystalline polymers — •Tonghua Liu, Rose Mary Michell, Albrecht Petzold, and Thomas Thurn-Albrecht — Von-Danckelmann-Platz 3, 06120, Halle(Saale)

The intracrystalline chain dynamics (ICD) plays a significant role in semi-crystalline polymers (SC), influencing not only the polymer crystallization and morphology but also the stability of crystals and the mechanical properties, such as drawability. Here we investigate how the ICD affects the stress relaxation of SC polymers.
Plane-strain compression test is used to study the relaxation behavior after yielding point. For crystal-fixed polymers like polycaprolactone (PCL), where ICD is absent or significantly hindered, only one relaxation process is observed. In contrast, crystal-mobile polymers like high density polyethylene (HDPE) exhibit two distinct relaxation processes, which can be attributed to the additional mobility within the crystals. The two relaxation processes in HDPE demonstrate markedly distinct time scales. The faster relaxation process is observed to relax faster with increasing temperature, whereas the slower relaxation process remains unaltered within the chosen temperature range.

CPP 15.56 Mon 19:00 P4

The effect of the intracrystalline chain diffusion on the non-linear mechanical behavior of semicrystalline polymers — •Rose Mary Michell, Albrecht Petzold, and Thomas Thurn-Albrecht — Martin Luther University Halle Wittenberg, Institute of Physics, D-06099 Halle, Germany.

This work studies the influence of intracrystalline chain diffusion (ICD) on the mechanical properties of semicrystalline polymers by comparing PEO with fast ICD and PCL with slow ICD. Mechanical tests were performed under plane strain compression at temperatures from -10 to 55 °C and true strain rates from 0.005 to 10 min^{-1}. At large deformations, the PCL always shows a strain hardening effect, while PEO shows softening when the rate decreases, temperature increases, and molecular weight decreases. The data corresponding to the strain hardening part, which describes the network forces, was fitted using the Gaussian model. The stress-strain curve for PCL showed higher stress than the Gaussian chain model predicted. In contrast, PEO had lower stress values; this difference could be attributed to an effect linked to chain mobility. For slow ICD, the crystals act as physical crosslinking points. Otherwise, the chains can be pulled from the crystals and soften the network. In conclusion, we found systematic differences in non-linear mechanical behavior between crystal-fixed and crystal-mobile polymers. This suggests that the competition between ICD and deformation determines the non-linear mechanical behavior at large deformations of semicrystalline polymers.

CPP 15.57 Mon 19:00 P4

Exploring the role of defects in polymer networks through simulations of 4-armed polymers — •Sayam Bandyopadhyay[1,2], Sebastian Seiffert[3], and Arash Nikoubashman[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01069 Dresden, Germany — [3]Department of Chemistry, Johannes Gutenberg Universität Mainz, 55128 Mainz, Germany

We simulated polymer networks formed by coarse-grained tetra-PEG (tPEG) macromolecules to investigate the effects of (connectivity) defects on network dynamics. We modeled both homoleptic and heteroleptic systems, where we modeled non-covalent bonds between functionalized end groups using an inverted Gaussian potential to control valency. The network structure was quantified through the fraction of bonded end groups and the radial distribution functions of attractive beads. Polymer mobility was characterized by examining the mean square displacement of individual tPEG molecules after gelation. To explore the impact of defects, we systematically altered the defect density by incorporating tPEG chains with inert end groups in the homoleptic systems and by varying the stoichiometry in the heteroleptic mixtures. Additionally, we examined how the bending stiffness of the polymers influenced network structure and dynamics, finding a marked slowing down with increasing stiffness. These findings provide new insights into the factors governing the role of defects in the structure and dynamics of polymer networks.

CPP 15.58 Mon 19:00 P4

Silicone implementation to car industry — •Yury Ostretsov — Moscow, Russia, Bolshaya Semenovskaya 38

Silicone is a preferred material for manufacturing automotive hoses due to its high heat resistance, resistance to aggressive chemical environments, flexibility, and durability. These properties allow silicone hoses to maintain shape and performance under extreme temperatures and pressure fluctuations, reducing the risk of leaks or failures. Additionally, silicone is lightweight compared to rubber alternatives, contributing to overall vehicle efficiency. Its ability to withstand ozone and UV exposure also enhances longevity, making it a reliable choice for various automotive applications.

CPP 15.59 Mon 19:00 P4

Water flow decrease of track-etched polyethylene terephthalate membranes in filtration applications — •Ana Ambroz[1,2], Zhen Yao[2], Christopher Rojas[3], Polina Angelova[2], Irena Petrinic[1], and Armin Gölzhäuser[2] — [1]Univeristy of Maribor, Maribor, Slovenia — [2]University of Bielefeld, Bielefeld, Germany — [3]CNM Technologies GmbH, Bielefeld, Germany

Track-etched (TE) membranes, with their precise pore size, controlled porosity, and defined pore geometry, are industrially applied as highly sensitive and fast filters for bacteria in the food, cosmetic and pharmaceutical industries, as control barriers in glucose sensors, and as biomolecule selective barrier in implants. Additionally, they are being investigated for their potential in reverse and forward osmosis for water purification and cold concentration. However, their tendency to lose performance over time presents a significant challenge, particularly in high-throughput and durable applications. In this work, we evaluate the performance of track-etched polyethylene terephthalate (TE-PET) membranes as nano- and microfilters in low-pressure reverse osmosis (LPRO) and dead-end filtration systems. Monitoring water flux through the TE-PET membranes at different low pressures (0.02-10 bar) revealed a gradual decrease over time, varying with porosity and pore size. Specifically, membranes with low porosity (<1.5%) and small pore sizes (<1.5 um) exhibited a significant reduction in water flux. The decline is attributed to membrane swelling and the formation of a sol-gel film within the pores, with additional contributing factors discussed.

CPP 15.60 Mon 19:00 P4

Intermolecular bonds - connecting structure and dynamics — •Martin Tress[1], Friedrich Kremer[1], and Jan Philipp Gabriel[2] — [1]Peter-Debye-Institute for Soft Matter Research, Leipzig University, Leipzig, Germany — [2]Institute of Materials Physics in Space, German Aerospace Center, Köln, Germany

Descriptions of the glass transition often consider temperature dependent changes in the specific volume to explain the tremendous increase in relaxation time, and empricial data confirm the general role of thermal expansion [Nat Phys 19 (2023) 694]. However, since glassy dynamics happens on molecular scale, macroscopic thermal expansion might be too coarse. Here we use infrared spectroscopy data to extract intermolecular hydrogen (H)-bond lengths in wide temperature ranges. For water, the H-bond expansion coefficient differs strongly from the macroscopic one, which is easily assigned to considerable structural reorganization in the water network [JCP 160 (2024) 234502]. Their comparison reveals that the most compact molecular arrangement is formed in the range ~316-331 K (i.e. well above the density maximum). This coincides with several pressure-related anomalies which confirms this characteristic point in the supra-molecular arrangement. These results confirm our earlier approach to deduce inter-molecular H-bond lengths in polyalcohols [JCP 154 (2021) 024503] and open a new alley to investigate the role of inter-molecular expansion as a precursor to structural relaxation on a bond-specific level.

CPP 15.61 Mon 19:00 P4

Single-molecule spectroscopy of organic laser gain media — •Janne Becker, Robert Schmidt, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics, University of Münster, Germany

Since the first experiments on pentacene [1], single-molecule spectroscopy has been performed for applications ranging from cell biology and medicine to organic laser media and single-photon emission [2]. To design and use these specialized molecules, their photophysical properties have to be investigated. Here, we perform single-molecule spectroscopy to study organic laser gain media. To isolate single molecules, we dilute the organic material down to concentrations of the order of nmol/L with ultra-pure solvents and measure characteristic fluorescence lifetimes and spectra.

References:

[1] W. E. Moerner and L. Kador, Physical Review Letters, 62, 2535. (1989)

[2] H. Miller et al, Rep. Prog. Phys. 81 024601 (2018)

CPP 15.62 Mon 19:00 P4

XPS study of redox mechanism in $Na_{2.5-x}Fe_{1.75}(SO_4)_3$ cathode material for high-voltage sodium-ion batteries — •Neama Imam[1], Karsten Henkel[1], Anna Milewska[2], Janina Molenda[2], Ehrenfried Zschech[1], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]AGH University of Krakow, Faculty of Energy and Fuels, Krakow, Poland

A multiplet splitting model based on the original work by Gupta and Sen has been used to track the redox mechanism and electronic structure of $Na_{2.5-x}Fe_{1.75}(SO_4)_3$, a high-performance cathode material for sodium-ion batteries (SIBs). This high-purity, off-stoichiometric open-channel cathode material with a tailored sodium-ion distribution, synthesized using an optimized solid-state route, demonstrates a high operating voltage of ∼3.8 V, surpassing the values reported for other cathode materials in the literature. X-ray photoelectron spectroscopy (XPS) was employed to analyze the evolution of the material's electronic structure at various charging potentials. Fe2$p_{3/2}$ spectra decomposition using the multiplet splitting model revealed the gradual oxidation of Fe^{2+} to Fe^{3+} during battery charging while transitioning from its pristine state ($x = 0$) with the presence of only Fe^{2+} at the cathode surface to the highest sodium de-intercalation level ($x = 1.61$). This result is consistent with the electrochemical analysis.

CPP 15.63 Mon 19:00 P4

Multiscale dynamics simulations of amorphous polyethylene terephthalate — •Andoni Ugartemendia[1], Alessandro Mossa[2], and Giorgia Brancolini[3] — [1]Institute of Nanoscience, CNR-NANO S3, via G. Campi 213/A, 41125 Modena, Italy — [2]Institute of Nanoscience, CNR-NANO S3, via G. Campi 213/A, 41125 Modena, Italy — [3]Institute of Nanoscience, CNR-NANO S3, via G. Campi 213/A, 41125 Modena, Italy

In the last decades, multiwall polymers have become widely used in food packaging due to their excellent mechanical and barrier properties. Unfortunately, the recycling of these materials is difficult and costly, leading to environmental problems. An understanding of the polymers properties is crucial towards the development of new recycling technologies. However, their computational modeling poses a great challenge since the dynamics span over several time scales. As a result, a multiscale approach becomes mandatory to gain access to the slower degrees of freedom. In this regard, coarse grained (CG) models have drawn considerable attention recently. CG models neglect the fastest degrees of freedom, flattening the rugged potential and thus, allowing higher time steps. In this work, we adopt a multiscale protocol to characterize several properties of polyethylene terephthalate (PET). First, atomistic molecular dynamics (MD) simulations are performed for amorphous PET systems with varying chain lengths. Then, the atomistic data is employed to derive a CG force field based on the iterative Boltzmann inversion (IBI). Finally, the structural data obtained with atomistic and CG simulaions are compared.

CPP 15.64 Mon 19:00 P4

Fourth-Generation High-Dimensional Neural Network Potentials for Molecular Chemistry in Solution — •Djamil Abdelkader Adel Maouene[1,2], Moritz Richard Schäffer[1,2], Moritz Gubler[3], Stefan Goedecker[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]Department Physik, Universität Basel, Switzerland

Machine learning has become a powerful tool in chemistry and materials science, as high-dimensional neural network potentials (HDNNPs) provide accurate representations of multidimensional potential energy surfaces for atomistic simulations. In this study, we compare the performance of two types of HDNNPs; 2G-HDNNPs and 4G-HDNNPs, in modeling organic molecules in aqueous solution. While 2G-HDNNPs have proven effective in many systems in capturing local interactions based on atomic environments, they fail in scenarios where long-range charge transfer plays a critical role. These cases are better addressed by 4G-HDNNPs, which take into account atomic charge variations caused by structural or electronic changes even at distant regions in the system. Both methods are demonstrated using a model organic molecule.

CPP 15.65 Mon 19:00 P4

Insights into Machine Learning Interatomic Potentials for simple analytical model systems — •Mirko Fischer and Andreas Heuer — Institute for Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster

During the past 10 years Machine Learning interatomic potentials

(MLIP) have gained popularity for Molecular Dynamics simulations with quantum chemical accuracy. Although it is a rapidly evolving field, many questions remain open. These include issues of interpretability, modeling different interaction types and how to select training data properly. MLIPs are rarely applied to simple model systems, for which the interactions of particles can be described analytically, to investigate these questions. Instead, MLIPs are mostly applied directly to realistic molecular systems for which the ground truth interactions must be approximated by methods like Density Functional Theory. By training an Atomic Cluster Expansion as a systematic and generally interpretable model for a Lennard-Jones model system, we aim to study how interaction types, system size and temperature affect the learned model in a systematic manner. The obtained interactions can be directly compared to the known true analytical interactions. Moreover, we fit a MLIP for an amorphous silica system to study structure and dynamics in a glass-forming system, where low-energy states are important. The question emerges, how to select the training data best and if such low-energy (low temperature) states must be explicitly included in it or if the MLIP is able to extrapolate from high-energy (high temperature) states to low energy states.

CPP 15.66 Mon 19:00 P4

Efficient Millisecond Timescale Modeling of Hydroxide Ion Dynamics in Aqueous Systems: A Multiscale Simulation Approach — •Jonas Hänseroth[1,2], Daniel Sebastiani[2], and Christian Dressler[1] — [1]Theoretical Solid State Physics, Institute of Physics, Ilmenau Universitiy of Technology, Ilmenau, Germany — [2]Theoretical Chemistry, Institute of Chemistry, Martin-Luther-University of Halle-Wittenberg, Halle (Saale), Germany

An adapted combined Molecular Dynamics/Lattice Monte Carlo (cMD/LMC) approach models hydroxide ion transport across extended systems and millisecond timescales.[1] The method surpasses classical Molecular Dynamics in efficiency while maintaining the accuracy of ab initio Molecular Dynamics, allowing the study of aqueous potassium hydroxide systems over a wide concentration range (3-61 wt.-%). The cMD/LMC algorithm allows simulations involving thousands of atoms at low computational cost, yielding diffusion coefficients consistent with ab initio benchmarks. This framework can provide insights into the dynamics of hydroxide ion in systems such as anion exchange membranes, which are essential for fuel cell technology. [1] J. Chem. Theory Comput. 2014, 10, 10, 4221-4228

CPP 15.67 Mon 19:00 P4

Confinement-induced dynamics in binary liquid mixtures: insights from molecular simulations — •Anam Sara, Pascal Merle, Siegfried Stapf, and Christian Dressler — Technische Universität Ilmenau, Germany

In this work, we investigate the behavior of binary liquid mixtures confined within silica nanopores, examining how confinement impacts the diffusion and relaxation properties of mixtures such as cyclohexane/acetone, cyclohexane/tetrahydrofuran (THF), water/acetone, and water/THF [1]. Experimental NMR measurements revealed deviations in diffusion coefficients and relaxation times of these mixture under confinement [2,3]. To interpret these observations, we perform molecular dynamics (MD) simulations to get atomistic insights into the structure and dynamics of these mixtures within the pores. Our primary objective is to characterize how confinement alters the microphase separation, component density distribution along the pore axis, and preferential interactions with pore walls.

[1] G. Guevara-Carrion, T. Janzen, Y. Muñoz-Muñoz, J.Vrabec, The Journal of Chemical Physics, 144, (2016).

[2] D. Bellaire, H. Kiepfer, K. Münnemann, H. Hasse, J. Chem. Eng.Data, 65, 793-803 (2020).

[3] Stapf, S., Siebert, N., Spalek, T., Hartmann, V., Gizatullin, B., and Mattea, C. (2023).

CPP 15.68 Mon 19:00 P4

Density of states in hard disks: Concentration dependency via SAMC simulation — Timur Shakirov[1,2], Malte Kautzsch[1], and •Viktor Ivanov[1] — [1]Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany — [2]Indivumed GmbH, Hamburg, Germany

We propose a new variant of SAMC sampling for determining the density of states as a function of the concentration of particles. The system is modelled as a set of dimensionless points, i.e., points with zero diameter. The minimal points separation, d_{min}, is chosen as the sampling parameter determining the macrostate. Thus, the density of states and the visiting histogram depend on the minimal distance d_{min} and are accumulated at each step of the algorithm according to the standard SAMC procedure. In a microstate (particular configuration of points' positions) with a given value of the minimal distance between points, d_{min}, one can replace the points with the hard disks of the diameter d_{min} (or less). This creates a system with a specific value of the concentration φ. We apply this algorithm for the two-dimensional system of hard disks to study its phase behaviour at different concentrations and compare the results with KTHNY theory and the previous simulations.

CPP 15.69 Mon 19:00 P4

Multiscale Simulation Framework for Functional Polymer Systems — •Steffen Kampmann[1], Alexander Croy[2], Arezoo Dianat[1], and Gianaurelio Cuniberti[1,3] — [1]Institute for Materials Science and Max Bergmann Center for Biomaterials, TU Dresden — [2]Chair of Theoretical Chemistry, Institute of Physical Chemistry, Friedrich Schiller University Jena — [3]Dresden Center for Computational Materials Science (DCMS)

Functional, mechanically resilient polymer and polymer-based nanocomposite films play an important role for strain gauges or organic light-emitting diode (OLED) displays [1-3]. The modelling and simulation workflow presented here enables the generation of disordered polymer systems and the linking of the mechanical and electronic properties from the atomistic to the microscopic size scale. Here, the focus is on the relationship between deformation and conductivity behavior. To calculate the multi-scale material behavior, we use density functional tight binding (DFTB) calculations, molecular dynamics simulations, and the finite element method. The in-situ processing, evaluation as well as the exchange of the generated data across simulation methods is performed using our Python framework. The multi-scale computational workflow indicated here represents a computationally efficient assessment of the properties of the polymer systems at different scales. [1] K. Grabowski, et al., Computational Materials Science, 135, 169*180, (2017) [2] R. Luo, et al., Progress in Organic Coatings, 162, 106593 (2022) [3] L. Liu, et al., Organic Electronics, 89, 106047 (2021)

CPP 15.70 Mon 19:00 P4

Investigation of electrolyte dynamics with interfaces: Insights from simple MD-models — •Katharina Kintrup[1,2], 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

Molecular Dynamics (MD) simulations are a common tool to investigate transport properties of electrolytes. Typically, periodic boundary conditions (pbc) are applied to simulate energetically closed systems, which are contrary to experimental systems with interfaces. Electrophoretic NMR (eNMR) experiments show that the incompressibility is dominating the transport properties of electrolytes, leading to an application of local conservation of volume. [1] Inspired by this, we set up simplified models to simulate binary liquids, imitating ionic liquids (IL), within interfaces, resulting in energetically open systems. After applying external (electric) fields, various properties of the model systems such as average velocities, number densities, volume densities, etc. were evaluated. A transition from local conservation of momentum towards local conservation of volume was observed. The velocities of all systems portrayed oscillations due to sound waves. A general analysis of dynamic processes on different time scales for systems without explicit charges was achieved. A comparison between systems with and without explicit charges was conducted, proving the superiority of the advanced charged model due to higher incompressibility. [1] J. Phys. Chem. Lett, 2022, 13, 8761-8767

CPP 15.71 Mon 19:00 P4

Evidence for unusual solvation shell of aqueous Fe^{3+} at high dilution — •Amrita Goswami, Elvar Örn Jónsson, and Hannes Jónsson — Science Institute and Faculty of Physical Sciences, University of Iceland, VR-III, 107 Reykjavík, Iceland

Solvated Fe^{3+} in water is a particularly important system, relevant, for instance, for the widely studied charge transfer Fe3+/Fe2+. However, the solvation shell of such highly charged cations is still poorly understood, particularly at for concentrations less than 1 M. In this regime of high dilution, experimental data and high-level calculations are sparse. For instance, most density-functional theory calculations are performed at a concentration of 0.8 M or higher, with uniform background charge. Simulations for such dilute solutions can provide insight inaccessible to other techniques. Using extensive molecular dynamics simulations with empirical potentials and DFT geometry optimizations of selected configurations, we study the effect of solution concentration on the solvation structure of aqueous Fe^{3+}. The solvation shell is found to undergo abrupt transitions between two states: an octahedral (OH) state with 6-fold coordination, and a metastable capped trigonal prism (CTP) state with 7-fold coordination. Further, we have developed a QM/MM (quantum-mechanical/molecular mechanical) method to study dilute solutions of aqueous Fe^{3+} with DFT-level accuracy, with a polarizable water model. References: Goswami et al., J. Phys. Chem. Lett., 2024

CPP 15.72 Mon 19:00 P4

Exploring Pathways of Supramolecular Self-Assembly at Liquid-Liquid Interfaces — •Mephin Philip Alamcheril[1], Friederike Schmid[1], and Shikha Dhiman[2] — [1]Institute for Physics, Johannes Gutenberg University Mainz — [2]Department of Chemistry, Johannes Gutenberg University Mainz

A self-assembly process usually occurs through thermodynamic pathways but the co-existence of different intermediates and diverse pathways of self-assembly have been observed. Liquid droplets are one such intermediate in many self-assembly processes, particularly in biological systems, which form through liquid-liquid phase separations (LLPS). Even though LLPS is a very well-known phenomena in polymer chemistry, only little is known about the possible role of LLPS in synthetic small molecule-based self-assembly.

In this project, we aim to study the possible mechanism of self-assembly at the surface of phase separated liquid droplets to explore the structure and dynamics at various stages of self-assembly and provide insights into how it can be controlled and manipulated for various applications. To that end, we develop a simple coarse-grained model for monomers in explicit solvent that self-assemble into fibers. The model is designed to represent BTA-like molecules in water. It is able to capture key characteristics of the experimental system such as the competition of fibril formation and liquid-liquid phase separation. We use it to examine the pathways of fibril formation from phase separated droplets.

CPP 15.73 Mon 19:00 P4

Isoconversional effect in epoxy polymerization process — •Sampanna Pahi[1], Christian Wick[1,2], and Ana Sunčana Smith[1,2,3] — [1]PULS Group, Institute for Theoretical Physics , FAU Erlangen-Nürnberg, Germany — [2]Group of Computational Life Sciences, Division of Physical Chemistry, Ruder Bošković Institute, Zagreb, Croatia — [3]Competence Unit for Scientific Computing (CSC), FAU, 91058 Erlangen, Germany

Isoconversional methods are essential for understanding the kinetics and predicting thermodynamic data in epoxy polymerization. While these methods have been experimentally validated, their computational modeling remains underexplored. In this study, we use molecular dynamics (MD) simulations and Quantum Mechanics/Molecular Mechanics (QM/MM) transition state (TS) analyses to investigate mechanisms and energetic barriers in epoxy thermoset curing, focusing on isoconversional effects. We generated post-a-priori QMMM reactive sites with hydrogen-bonded systems to examine the influence of hydrogen bonding on the curing process. Initial results without hydrogen bonds showed higher activation energies than experimental values, with some outliers showing lower energies. Adding hydrogen bonds, especially hydroxyl (OH) bonds, reduced activation energies and explained these discrepancies. Radial distribution function (RDF) analyses showed OH bond formation is more likely than amine (NH) bonds, highlighting hydrogen bonding*s critical role in isoconversional effects during epoxy curing.

CPP 15.74 Mon 19:00 P4

A Multiscale MD-QM/MM Approach for Modeling Fracture Behavior in Epoxy Resins — •Barişcan 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 Physical Chemistry, Ruder Bošković Institute 10000 Zagreb, Croatia

Epoxy resins, with their exceptional mechanical properties, are indispensable in advanced engineering applications. However, understanding their fracture behavior at the molecular level remains a challenge. This study presents a multiscale framework that couples molecular dynamics (MD) simulations with quantum mechanics/molecular mechanics (QM/MM) calculations to analyze bond rupture and crack propagation in epoxy networks. The MD component monitors strain accumulation and identifies critical bond elongation thresholds indicative of imminent fracture. When these thresholds are met, the simulation transitions to QM/MM calculations, where bond breakage is determined dynamically by considering the surrounding chemical environment. This on-the-fly approach enables efficient and accurate modeling of fracture events and their impact on larger-scale material behavior, providing a foundation for future studies of epoxy resin failure mechanisms.

CPP 16: Energy Storage and Batteries I

Time: Tuesday 9:30–11:15 Location: H34

Invited Talk CPP 16.1 Tue 9:30 H34

Multifunctional structural batteries — •Göran Lindbergh — KTH Royal Institute of Technology, Stockholm, Sweden

A multifunctional lightweight material combines several functions in a single material entity able to simultaneously bear mechanical loads by acting as a carbon fibre composite component while providing one or more other functionalities at the same time, e.g. storing energy. In this work, we will show functionalities coming from alkali ion insertion in carbon fibres that goes beyond the battery function, and how these functions can be combined in a single device.

The starting point for these concepts is so called structural batteries, which are multifunctional composite materials able to carry load while storing electrical energy like lithium-ion batteries. In such a battery, carbon fibres are used as the load carrying material thanks to their excellent strength and stiffness properties, but also as the active negative electrode. They also include a multifunctional matrix system, a structural battery electrolyte (SBE), the material holding the fibres together to make a solid-state load carrying material, but which at the same time is ionically conductive and chemically stable. It includes a multifunctional positive electrode, a composite electrode based on conventional ion inserting materials like lithium iron phosphate (LFP) supported by electrochemically active carbon fibres for load carrying and electrical conduction. This device can then also be used for inherent strain sensing in the material and can also be made to shape-morph with electrical control at low voltages and for harvesting energy by converting mechanical strain to electrical power.

CPP 16.2 Tue 10:00 H34

Structural response of advanced silicon-containing graphite anodes in commercial Li-ion batteries — •Tobias Hölderle[1,2], Dominik Petz[1,2], Vladislav Kochetov[2], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]MLZ, TUM, 85748 Garching, Germany

This study explores the structural behavior of graphite anodes containing silicon additives in commercial lithium-ion batteries (LIBs) through detailed X-ray and neutron powder diffraction analyses. Silicon is increasingly utilized in advanced LIB anodes due to its potential to significantly increase energy capacity. However, its substantial volume expansion and amorphization during lithiation, complicate direct observation of lithium redistribution within the anode via diffraction techniques. Nonetheless, an indirect structural response linked to the lithiation of silicon was identified, indicated by a delayed lithium intercalation into the graphite structure. Furthermore, aging effects on high-silicon-content anodes were explored, showing the role of silicon in accelerating electrode degradation over time. These findings enhance our understanding of the complex relationship between the silicon content in the anode, structural stability, and lithium transport in advanced LIBs.

CPP 16.3 Tue 10:15 H34

XPS study of redox mechanism in Na2.5-xFe1.75(SO4)3 cathode material for high-voltage sodium-ion batteries — Neama

Imam[1], •Karsten Henkel[1], Anna Milewska[2], Janina Molenda[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]AGH University of Krakow, Faculty of Energy and Fuels, Krakow, Poland

A multiplet splitting model based on the original work by Gupta and Sen has been used to track the redox mechanism and electronic structure of Na2.5-xFe1.75(SO4)3, a high-performance cathode material for sodium-ion batteries (SIBs). This high-purity, off-stoichiometric open-channel cathode material with a tailored sodium-ion distribution, synthesized using an optimized solid-state route, demonstrates a high operating voltage of ~3.8 V, surpassing the values reported for other cathode materials in the literature. X-ray photoelectron spectroscopy (XPS) was employed to analyze the evolution of the material's electronic structure at various charging potentials. Fe2p3/2 spectra decomposition using the multiplet splitting model revealed the gradual oxidation of Fe2+ to Fe3+ during sodium de-intercalation while transitioning from its pristine state with the presence of Fe2+ at the cathode surface only to the fully charged state (Na0.89Fe1.75(SO4)3 at 4.5 V). This result is consistent with the electrochemical analysis.

CPP 16.4 Tue 10:30 H34

Multipoint Anionic Bridge: Asymmetric Solvation Structure Improves the Stability of Lithium-Ion Batteries — •Tianle Zheng[1], Ya-jun Cheng[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Ningbo Institute of Materials Technology & Engineering, Chinese Academy of Sciences, Ningbo, 315201, Zhejiang Province, P. R. China

In this study, a novel concept of multipoint anionic bridge (MAB) is proposed and proved, which utilizes anions with different sites to connect with the asymmetric solvation structure (ASS). Compared to usual solvation structures, this study uses the multifunctional groups of difluoro(oxalate)borate anion, which can connect with Li ions. By tailoring the concentration, the anion serves as a bridge between different solvated structures. In-situ techniques and simulations investigate electrolytes to draw correlations between solvation structures and reaction pathways. The proposed design demonstrates remarkable high-temperature performance on both the anode and cathode sides, enabling stable cycling of lithium cobalt oxide (LCO)||graphite (0.5 Ah, 1.0 C) pouch cell for over 200 cycles at 80 °C, and facilitating Li||MCMB and Li||lithium iron phosphate (LFP) cells to deliver stable performance for 200 cycles at 100 °C. This work paves a way to develop high-performance electrolyte systems by designing and using new multipoint anions to construct ASSs.

CPP 16.5 Tue 10:45 H34

In situ Mechanochemical Synthesis of Organic Anodes in Electrode Processing for Ultra-long Sodium Storage — •Ying Qi, Huaping Zhao, and Yong Lei — TU Ilmenau

Currently, hard carbon is commonly used as an anode material in sodium-ion batteries (SIBs). However, hard carbon anodes face several challenges, including time-consuming and energy-intensive synthesis processes, low-voltage operating platforms, and capacity storage with a steep slope. These issues contribute to severe dendrite growth and reduced full-cell capacity, negatively affecting electrochemical performance. In contrast, organic anodes are becoming a focal point in SIBs research due to their abundant availability, low cost, simple synthesis, and stable potential plateaus. In this study, we directly prepared a series of acid anhydrides including perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA), 1,4,5,8-naphthalenetetracarboxylic dianhydride (NTCDA), and pyromellitic dianhydride (PMDA) into electrodes using a one-step milling process during slurry preparation. The prepared Na4PTC electrodes show low potential plateaus and ultra-stable cycling performance in SIBs. It exhibited exceptional performance, demonstrating ultra-long cycling stability lasting nearly one year. Additionally, the assembled full cell delivered a high energy density of ~200 Wh kg-1.

CPP 16.6 Tue 11:00 H34

Localized highly concentrated electrolytes with perfluorocarbonate diluents enable high-energy-density lithium/sodium metal batteries — •Zhuijun Xu[1], Yinghui Li[2], Yajun Cheng[2], Yonggao Xia[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Ningbo Institute of Materials Technology & Engineering, Chinese Academy of Sciences, Ningbo, Zhejiang, 315201, P. R. China

Localized high-concentration electrolytes (LHCEs) have been widely recognized for their critical role in managing the reversible plating/stripping of alkali metals. multi-functional diluents with more stable physical and chemical properties are crucial for enhancing battery performance and safety. In this study, a variety of solvents, including 4-fluoro-1,3-dioxolan-2-one, 4,4-difluoro-1,3-dioxolan-2-one, cis-4,5-difluoro-1,3-dioxolan-2-one, trans-4,5-difluoro-1,3-dioxolan-2-one, 4,4,5-trifluoro-1,3-dioxolan-2-one, and 4,4,5,5-tetrafluoro-1,3-dioxolan-2-one, were analyzed using Density Functional Theory (DFT) calculations. Further, molecular dynamics (MD) simulations were conducted on the aforementioned solvents and their corresponding LHCEs for lithium/sodium metal batteries (LMBs/ SMBs). A comprehensive set of physical and chemical properties was examined, including the density of the solvent molecules, their highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies, and their binding energies with lithium or sodium ions, distinct solvation structures within various LHCEs.

CPP 17: Modeling and Simulation of Soft Matter I

Time: Tuesday 9:30–11:15 Location: H38

Invited Talk CPP 17.1 Tue 9:30 H38

Continuum models for water's peculiar behavior on the nanoscale — •Alexander Schlaich — Institute for Atomistic Modeling of Materials in Aqueous Media, Hamburg University of Technology, Germany

Water at the nanoscale exhibits unexpected properties relevant to many soft matter applications, ranging from the hydration forces that stabilize biological matter, via interfacial viscous effects that dominate wear behavior, to the unique dielectric behavior. Atomistically, these effects can be linked to the strong hydrogen bonding network and the corresponding water orientation and density at interfaces and in confinement – observables directly accessible from molecular simulations. However, relating these properties to experimental, typically macroscopic or at least averaged quantities is a tedious task. Here I will discuss some of the progress we have made in the last few years in deriving effective descriptions of the microscopic details that can be used to apply continuous descriptions and thereby extract, for example, experimentally accessible hydration pressure, permeance, or capacitance. Our recent work has focused on combining concepts from solid state theory and soft matter physics to accurately treat the electrode/electrolyte interface, and I will present our analysis of the unusually high capacitance of pure water capacitors.

CPP 17.2 Tue 10:00 H38

Coupled self and collective dynamics in highly charged colloidal Yukawa-systems — •Daniel Weidig and Joachim Wagner — University of Rostock, Rostock, Germany

We investigate binary mixtures of highly charged colloidal particles employing Brownian dynamics simulations. In mixtures of identically charged, but differently sized particles solely the Stokes-Einstein diffusion coefficients differ, while the interactions are practically size-independent. Due to these identical interactions the static structure of all species are identical and independent on dynamical properties of the particles, as observed in partial static pair correlation functions. A dynamical coupling of both self and collective motion is observed in these systems. The long-time self-diffusion coefficient of a larger species is enhanced by the presence of a smaller, more mobile species and vice versa. Similar coupling effects are as well observed in the initial correlation decay of partial, distinct intermediate scattering functions, quantified by relaxation rates and stretching exponents of stretched exponentials. For all the here mentioned parameters, in the limit of strongly electrostatically coupled colloidal systems in first approximation linear dependencies on the size-ratio and reduced number density are observed. Despite we investigated highly dilute colloidal suspensions, where normally hydrodynamic interactions are neglectable, we found especially in binary mixtures an enhancement of the self and collective diffusion coefficients due to hydrodynamic interactions. Contrary, in one-component systems, hydrodynamic interactions do not have significant influence on time-dependent diffusion coefficients.

CPP 17.3 Tue 10:15 H38

Grand canonical molecular dynamics simulation of surface-initiated polymerization — •Bhuwan Poudel and Kurt Kremer — Max Planck Institute for Polymer Research, Mainz, Germany

The post-characterization of polymer brushes prepared from surface-initiated polymerization (SIP) is challenging because of their unique morphology and limitations in experimental techniques. However, in simulation counterparts, it is much easier to gain control over SIP processes. In this work, we used grand canonical molecular dynamics simulations to investigate the growth kinetics and characterization of polymer brushes. The SIP was studied by varying the grafting density. At low grafting densities, nearly monodisperse brushes were obtained. The dispersity was found to be increased with increasing grafting density; as a result, brushes with broad molecular weight distribution were obtained. We also showed that parameters such as thickness, molecular weight, and dispersity can be precisely controlled during SIP. The results suggests that the method presented here provides strategies to synthesize polymer brushes and tailor their properties more efficiently.

CPP 17.4 Tue 10:30 H38

IR Spectroscopy and Electric Field Simulations Enabled by the Atomic Polar Tensor Neural Network — •Philipp Schienbein — Lehrstuhl für Theoretische Chemie II, Ruhr-Universität Bochum, 44780 Bochum, Germany — Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, 44780 Bochum, Germany

Vibrational spectroscopy is a vital technique for uncovering microscopic structure and dynamics of condensed phase systems. However, interpreting such spectra at the microscopic level often requires theoretical support. While ab initio molecular dynamics (AIMD) has proven effective for this purpose, its high computational cost – especially when using electronic structure methods beyond GGA DFT – can be prohibitive. We have recently introduced a machine learning molecular dynamics (MLMD) approach for accurately calculating IR spectra using the atomic polar tensor, a size-intensive physical observable that can uniquely be defined for each atom and is thus broadly applicable across diverse systems. Notably, the atomic polar tensor also rigorously enables MLMD simulations under external electric fields. In this work, I benchmark this method against explicit AIMD simulations demonstrating comparable accuracy with significantly reduced computational cost and present applications of the atomic polar tensor neural network. These examples highlight its potential to drive novel physical insights, particularly in scenarios requiring large-scale MD simulations or computationally intensive electronic structure methods.

CPP 17.5 Tue 10:45 H38

Reducing dynamical helical polymers to 1D Ising models: long-range effects from polymer self-avoidance — •Keerti Chauhan[1], Marcus Müller[2], and Kostas Daoulas[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Georg-August-Universität Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany

Cooperative chiral order in dynamic helical polymers (DHP) is commonly understood by reducing them to 1D Ising chains. Each spin can switch between $\sigma = -1$ and $\sigma = +1$ to represent rapid interconvertion between left-handed (M) and right-handed (P) helical twist. Spins are ferromagnetically coupled to capture the energetic disadvantage of boundaries between P and M domains. Currently, all 1D Ising models of DHP assume nearest-neighbor (NN) spin-spin interactions. We use a minimal model to challenge this assumption and investigate whether polymer self-avoidance, due to excluded volume, leads to effective non-local coupling between spins. Polymers are represented by freely-jointed chains with reversible hinges and helicity is described by a NN 1D Ising Hamiltonian with coupling strength J. Ideal and self-avoiding DHP are generated via a Monte Carlo scheme. First, we verify that in ideal chains the spins reproduce the statistics of a NN 1D Ising model with coupling strength J. Next, we find that chain self-avoidance does create effective long-range interactions between spins, as demonstrated by spin-spin correlation functions and free-energy calculations. These interactions renormalize J and create finite-size effects that are inconsistent with a NN 1D Ising behavior.

CPP 17.6 Tue 11:00 H38

Stabilization of Sodium Dodecyl Sulfate Reverse Micelles in Acid Solutions and Toluene from Molecular Dynamics Simulations — •Qixuan Li — Ruhr University Bochum, Bochum, Germany

The anionic surfactant Sodium dodecyl sulfate (SDS) forms reverse micelles (RMs) in two non-miscible components above the critical micelle concentration. Although the RMs in salt or alkali solution has been investigated in previous studies, less is known on the working mechanism of acids in SDS RMs. Here, we employ all-atom molecular dynamics simulations using Generalized Amber Force Field (GAFF) to investigate the effects of chloroauric acid (HAuCl4), fluoroboric acid (HBF4), phosphoric acid (H3PO4) and perchloric acid (HClO4) solutions on the stability of the RMs through spontaneous self-assembly in toluene. We find that all kinds of acids can stabilize micellar structure, and in particular high concentration of acids can significantly enhance the stability of RMs. In addition, H2PO4- anions tend to accumulate close to the RM surface, because they can form stable hydrogen bonds with the sulfate-based headgroup of SDS molecules or hydrated protons. Our findings can help to rationalize the impact of different acids on the RMs stability and in turn on the metallic nanoparticles synthesis where the RMs are used as nanoreactors.

CPP 18: Biomaterials, Biopolymers and Bioinspired Functional Materials II (joint session CPP/BP)

Time: Tuesday 9:30–11:15 Location: H46

Invited Talk CPP 18.1 Tue 9:30 H46

Hybrid materials from colloidally stable nanocellulose and nanoparticles - scattering techniques are needed for characterization — •Eva Malmström[1], Åsa Jerlhagen[1], Benedikt Sochor[2], Korneliya Gordeyeva[1], and Stephan Roth[1,2] — [1]KTH Royal Institute of Technology, Stockholm, Sweden — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Cellulose nanofibrils (CNFs) have rendered increasing interest during the last decades as their high stiffness, strength, and aspect ratio are attractive features to further explore on the pathway to a more sustainable society.

Controlled radical polymerization procedures allow for the synthesis of well-defined, nearly monodisperse, block-copolymers. The development of the polymerization-induced phase self-assembled (PISA) technique enables the production of well-defined nanoparticles (nanolatexes), with controlled size (typically with a diameter smaller than 200 nm), charge density, chemical functionality, and glass transition temperature.

The combination of CNFs and well defined nanolatexes allows for the design of novel materials with unique properties. Scattering techniques have proven very useful to characterize the corresponding materials, for instance, a method to assess cross-section orientation.

CPP 18.2 Tue 10:00 H46

In situ GISAXS investigation of different protein-templated titania nanostructures — •Linus Fidelis Huber and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Nanostructured titania thin films have been studied for a large variety of applications. An environmentally benign and scalable synthesis route for this material class could be of interest to many state-of-the-art devices, from solar cells to battery materials. Protein-assisted sol-gel synthesis is a low-temperature, low-cost, and highly scalable technique, that can be used to achieve a nanostructured titania thin film. It has been shown that the bovine whey protein β-Lg forms differently shaped aggregates at different solution pH values. With simple changes to the solution chemistry, different domain sizes, porosities, and morphologies are possible. Therefore, it is a promising candidate to create tunable and mesoporous titania structures. In this work, we investigate the film formation with in situ small-angle/wide-angle grazing incidence X-ray scattering (GISAXS/GIWAXS) techniques. It is found that films printed at acidic pH form significantly different final bulk morphologies than films printed at neutral pH. The crystallite phase is strongly reduced in average domain size and domain-domain distance. Agglomerate size is increased for the acidic template. The in situ data is complemented by SEM, PL, UV-Vis and static GISAXS/GIWAXS measurements.

CPP 18.3 Tue 10:15 H46

With digital luminescence towards minimalistic, biodegradable information storage — •Sebastian Schellhammer, Heidi Thomas, Tim Achenbach, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Dresden, Germany

Materials showing persistent luminescence, characterized by extended excited state decay times in the millisecond range and beyond, have gained much attention. Recently, we have reported a photonic device architecture based on organic functional materials called programmable luminescent tag (PLT) that is well suited for sensing, labelling, and information exchange applications. Information can be erased and rewritten repeatedly by using the design principle of digital luminescence, i.e. the control of the local oxygen concentration in a polymer:emitter blend and accordingly the emission by room temperature phosphorescence (RTP). We present the design of PLTs made from industrially compostable, ready-to-use materials (bioPLTs). As natural emitters, quinoline alkaloids show sufficient RTP when being embedded in a polymer matrix. Polylactic acid is used as matrix material and flexible substrate. RTP can be controlled adding oxygen blocking layers made from Exceval. Although organic semiconductors provide the potential of biodegradable technologies, prototypes do only rarely exist. With this work, a promising technology for compostable information storage and sensing systems is introduced.

CPP 18.4 Tue 10:30 H46

Enhancing drug release at interfaces with photoresponsive surfactant-polyelectrolyte mixtures — •Ipsita Pani, Michael Hardt, and Björn Braunschweig — Institute of Physical Chemistry, Center for Soft Nanoscience (SoN), University of Münster, Corrensstraße 28-30, Münster 48149, Germany

Using micellar nanocarriers of a photoresponsive arylazopyrazole (AAP) surfactant, we have recently demonstrated the drug release at air-water interface.[1] In this work, we use a biopolymer poly-L-lysine (PLL) to form surfactant-polyelectrolyte mixtures to enhance the drug release of a chemotherapeutic drug doxorubicin. We observe a strong binding between the negatively charged AAP and the positively charged PLL at equimolar ratio. The information from UV-visible spectroscopy, light scattering studies, surface tensiometry and SFG spectroscopy has been utilized to identify the concentration of PLL at which the light-induced drug release is enhanced at the interface. We found that at higher PLL:AAP ratio, the complexes have low net charge and colloidal stability and the release of Dox from the bulk solution to the air-water interface is not observed. However, at lower PLL:AAP ratio, when the system is colloidally stable with a net negative charge, the drug release to the air-water interface is significantly enhanced. Further, the kinetics of drug release to the interface is faster in presence of PLL-AAP mixtures in comparison to pure AAP micelles. Reference : [1] Pani et al. Chem. Sci., 2024, 15, 18865-18871.

CPP 18.5 Tue 10:45 H46

Proteins as foam stabilizers: From single foam lamellas to macroscopic foams — •Kevin Gräff, Sebastian Stock, Luca Mirau, Matthias Kühnhammer, Olaf Soltwedel, and Regine von Klitzing — Terchnische Universität Darmstadt, Darmstadt, Germany

Foams consist of foam lamellas, which separate single air bubbles from each other. Investigation of lamellas is crucial to understand foam properties. In order to untangle electrostatic, steric and network stabilization effects, we compare two globular proteins (β-lactoglobulin and Lupine Protein Isolate) and a disordered, flexible protein (whole casein) at different pH values. The Thin Film Pressure Balance (TFPB) device based on image intensity measurements generates spatially resolved disjoining pressure isotherms. We introduce feature tracking for the measurement of interfacial mobility and stiffness of lamellas as a novel method. Around the isoelectric point, Newton Black Films (NBFs) form, which are stable for the globular proteins while they are unstable for the disordered flexible one. This difference in film stability is explained by different characteristics of network structures in the lamellas from the respective protein solutions. Small-Angle Neutron Scattering (SANS) evaluation with a new model for foams proves the presence of NBFs within macroscopic foams. For a complete picture we compare the TFPB findings with X-ray reflectometry as well as with Brewster Angle Microscopy on single interfaces.

[1] Gräff, K. et al, (2022), Untangling effects of proteins as stabilizers for foam films, Front. Soft. Matter 2:1035377.

CPP 18.6 Tue 11:00 H46

What makes a polysaccharide biomaterial a good candidate for tissue engineering applications? — •Emma Bobu Cimpoi[1], Codrut Costinas[1], Emilia Licarete[2], Tamás Gyulavári[3], Klara Magyari[4], and Monica Baia[4,5] — [1]Doctoral School of Physics, Babes-Bolyai University, Cluj-Napoca, Romania — [2]Centre for Systems Biology, Biodiversity and Bioresources "3B", Cluj-Napoca, Romania — [3]Department of Applied and Environmental Chemistry, University of Szeged, Hungary — [4]INSPIRE Research Platform, Babes Bolyai University, Cluj-Napoca, Romania — [5]Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania

Biomaterials are inovative systems used to solve medical issues. Daily, injuries produce major bleeding that affects people and, without proper care, leads to other health problems. Traditional care methods are limited and outdated, so the focus is on natural materials with hemostatic properties, that are biocompatible and non-toxic. The aim of this work was to develop biomaterials based on pullulan, alginate and gelatin in various combinations, which could stop the bleeding and regenerate the wound. The developed sponge-like materials were characterized by FT-IR spectroscopy and X-ray diffraction. Then they were evaluated in vitro in terms of porosity, toxicity, swelling and charge on the surface, using SEM, cell viability assays, water up-take and mechanical tests. The investigations revealed good results as the synthesis was succesfull, the samples swell a lot, have good shape memory properties, are porous and non-toxic. These indicate their potential to stop bleeding, and therefore further in vivo tests will be carried out.

CPP 19: Active Matter III (joint session DY/BP/CPP)

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

CPP 19.1 Tue 9:30 H47

From micro to macro: systematic coarse-graining of active particle models and implications on phase separation — •Sumeja Burekovic[1], Filippo De Luca[2], Cesare Nardini[1,3], Ananyo Maitra[4,5], and Michael E. Cates[2] — [1]CEA, Paris-Saclay, France — [2]DAMTP, University of Cambridge, UK — [3]LPTMC, Sorbonne Université, France — [4]LPTM, CY Cergy Paris Université, France — [5]LJP, Sorbonne Université, France

Significant insights into collective phenomena of active systems, such as phase separation, have been obtained through minimal field theories developed in a top-down manner. In contrast, the bottom-up approach seeks to link these continuum models to the microscopic dynamics of active particles, often formulated as Langevin equations for their position and orientation. This connection is typically achieved via explicit coarse-graining and allows active field theories to be expressed in terms of physically meaningful parameters. A major challenge in coarse-graining is the consistent elimination of irrelevant fast degrees of freedom to derive closed equations for the hydrodynamic variables or order parameters, such as the density field. We propose a systematic extension of standard homogenization/projection-operator techniques. As we show in minimal examples with few degrees of freedoms, our technique allows to go beyond the state of the art of homogenization in the mathematical literature. We then discuss the predictions of our coarse-graining methods for the large-scale phenomenology of non-aligning active particles, including cases in which microphase separation - rather than full phase separation - emerges due to activity.

CPP 19.2 Tue 9:45 H47

Active Quadrupolar Dumbbells — •Margaret Rosenberg[1], Marco Musacchio[1], Lorenzo Caprini[2], and Hartmut Löwen[1] — [1]Heinrich-Heine University Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf — [2]Università di Roma Sapienza, P.le Aldo Moro 2, 00185 Rome, Italy

The field of Active Matter has thrived in recent years, driven both by the insight that it underlies fundamental processes in nature, and by its vast potential for applications. Although the self-propulsion mechanisms of Active Matter allow us to consider and control a wide range of motions, there is - by default - no obvious control over the orientation and rotation of the particles. One approach to resolve this is the use of anisotropic particles and interactions. This contribution presents a computational study of a novel system composed of active, quadrupolar dumbbells, the phase behavior of which is determined by the competition between active motion and the orthogonal alignment favored by quadrupolar attraction. We explore the novel phase behavior unlocked by these anisotropic interactions, and discuss options for experimental realizations and applications.

CPP 19.3 Tue 10:00 H47

Order by disorder in a swarm with obstacles — Pradeep Kumar[1], Sanjay Puri[1], and •Martin Weigel[2] — [1]School of Physical Sciences, Jawaharlal Nehru University, New Delhi – 110067, India — [2]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Simple models of swarming and active matter such as the Vicsek model [1] have been studied in detail, and the phase diagram as a function of noise strength and particle density is by now well understood. Real active systems are usually affected by impurities and random disorder, however. The presence of a quenched distribution of disc-like obstacles in the domain of the Vicsek model is observed to have a dramatic effect on the ordering behavior [2]: in contrast to the model without obstacles, where the strongest alignment is observed for the lowest noise, as soon as obstacles are added only the presence of a certain amount of noise leads to a global alignment of particles. This order by disorder phenomenon for active systems is traced back to the interplay of multiple length scales in the system: the typical inter-obstacle distance, the typical cluster size, and the resulting mean-free-paths of cluster-obstacle and cluster-cluster collisions. We present scaling arguments explaining these connections and provide an outlook towards similar phenomena in related systems.

[1] T. Vicsek, Phys. Rev. Lett. 75, 1226 (1995).

[2] O. Chepizhko, E. G. Altmann, and F. Peruani, Phys. Rev. Lett. 110, 238101 (2013).

CPP 19.4 Tue 10:15 H47

Autonomous navigation in synthetic microswimmers: solving mazes with chemical echolocation — •Aritra K. Mukhopadhyay[1], Linhui Fu[2], Kai Feng[2], Ran Niu[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, Darmstadt, Germany. — [2]Huazhong University of Science and Technology, Wuhan, China.

Motile microorganisms like bacteria and algae combine self-propulsion, cooperation, and decision-making at the micron scale. Inspired by these biological systems, synthetic microswimmers are emerging as human-made counterparts capable of self-propulsion. Recent breakthroughs provide a platform to integrate additional functionalities, bridging the gap between biology and synthetic systems.

We propose and experimentally demonstrate a mechanism enabling synthetic microswimmers, such as autophoretic colloids, droplet swimmers, and ion-exchange-driven modular swimmers, to make autonomous navigational decisions. These swimmers generate chemo-hydrodynamic signals that interact with boundaries, creating echoes that carry structural information about the environment. Remarkably, these echoes invoke automatic responses, such as synthetic chemotaxis, enabling the swimmers to avoid dead ends and autonomously find paths through complex mazes.

Our findings illustrate how simple physical principles can endow synthetic systems with advanced navigation functionalities, which could be useful for developing self-navigating micromachines with potential applications in targeted drug delivery and environmental sensing.

CPP 19.5 Tue 10:30 H47

Active Particles in Tunable Colloidal Environments — •Abhimanyu Nowbagh[1], Venkata M.S.G. Tanuku[2], Thomas Palberg[2], and Ivo Buttinoni[1] — [1]Institute of Experimental Colloidal Physics, Heinrich-Heine University, 40225 Düsseldorf — [2]Institute of Physics, Johannes-Gutenberg University, 55128 Mainz

Active colloids are microscopic particles which propel through aqueous media by converting the externally available energy into directed motion. Using non equilibrium thermodynamics to understand biological systems: interactions of active colloids with crowded systems, and emergent phenomena of ensembles of active particles, remain an important and open question.

In this work, we investigate the dynamics of active particles in crowded environments subjected to alternating-current (AC) electric fields. The AC electric field is used to control: i) the velocity of active particles and ii) the inter-particle interaction between passive colloids. As we increase electric field strength, the velocity of active particles increases and the inter-particle interaction between passive colloids becomes stronger. We study the behaviour of active particles as a function of: i) the frequency of the applied AC electric field, ii) the area fraction of the passive crowd, iii) the active to passive particle number ratio, and iv) the velocity of the active particles.

Our experimental findings show that the active particles reorient faster with an increasing electric field strength. With an increase in the active to passive particle ratio, we show that cluster formation is non-monotonically sensitive to the passive crowd density.

Invited Talk CPP 19.6 Tue 10:45 H47

Beyond spheres - active matter in new shapes — •Juliane Simmchen — University of Strathclyde, Cathedral street 295, Glasgow UK

Surface minimisation for a given volume is energetically favourable on the small scale - this is why most colloidal particles are spherical. In active matter they have the added advantage of facilitating comparison between experiment and theory, one of the reasons why spherical Janus particles dominate the field.

However, broadening the range of materials has led to interesting discoveries - behaviour that would not have been observable in the spherical regime. This talk will give an overview of the intriguing behaviour of non-spherical active materials at the microscale - from plates to truncated bipyramids and rods.

15 min. break

CPP 19.7 Tue 11:30 H47

Modeling Filamentous Cyanobacteria — •Elias Fischer and Holger Stark — Institute Of Theoretical Physics, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Filamentous cyanobacteria play an important role in many ecosystems and the carbon cycle of our planet, both in the present and the past. They triggered the great oxygenation event about 2.5 billion years ago, generating the atmospheric oxygen of our planet while contributing large parts of our fossil fuel record.

Filamentous cyanobacteria exhibit gliding motility when in contact with solid surfaces or each other. Despite their ecological relevance and increased use in biotech applications, the exact nature of the force-generating process remains not fully understood. Furthermore, the gliding of cyanobacteria is strongly affected by external cues, most importantly light. They aggregate in regions with the highest light intensity, which means best environmental conditions for photosynthesis.

Following recent advances in understanding the self-organization of cyanobacteria, we present a novel approach for modeling the mechanical and behavioral aspects of individual cyanobacteria filaments, including force synchronization and response to light. Each filament is modeled as a bead-spring chain in 3D with bending and torsional elasticity, as well as a hard-core repulsion between the filaments. Notably, the propulsion forces that drive the individual parts of the filament forward are only considered locally where the filament comes into contact with another surface. First results on the 3D bending and twisting motion of a filament and its reaction to light are presented.

CPP 19.8 Tue 11:45 H47

Self-assembly and control of active and passive triblock Janus colloids — •Juri Franz Schubert, Salman Fariz Navas, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

Triblock Janus colloids belong to the family of patchy particles, interacting with hydrophobic attraction at opposite poles and electrostatic repulsion in the equatorial region. They are known to self-assemble into a colloidal kagome crystal from experiments [1] and theory [2,3,4]. However, investigating the self-assembly of such systems via Brownian Dynamics can result in timescales inaccessible to brute force simulations, often requiring complex sampling techniques [3]. Recently, it has been shown that introducing self-propulsion can significantly accelerate self-assembly and enhance the Kagome yield [4]. Here, we study the model introduced in [4] and further investigate the self-assembled structures in active and passive systems. Using simple time-dependent activity protocols, we are able to sample a temperature-density state diagram of the passive system. Our results closely match with earlier studies [2,3], where different triblock models and sampling techniques were used.

[1] Q. Chen, S. C. Bae, S. Granick, Nature 469, 7330 (2011).
[2] F. Romano, F. Sciortino, Soft Matter 7, 12 (2011).
[3] K. Bahri, H. Eslami, and F. Müller-Plathe, JCTC 18, 1870 (2022).
[4] S. A. Mallory, A. Cacciuto, JACS 141, 6 (2019).

CPP 19.9 Tue 12:00 H47

Enhanced Diffusion and Universal Rouse-like Scaling of an Active Polymer in Poor Solvent — Suman Majumder[1], Subhajit Paul[2], and •Wolfhard Janke[3] — [1]Amity Institute of Applied Sciences, Amity University Uttar Pradesh, Noida 201313, India — [2]Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India — [3]Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany

By means of Brownian dynamics simulations we study the steady-state dynamic properties of a flexible active polymer in a poor solvent condition. Our results show that the effective diffusion constant of the polymer D_{eff} gets significantly enhanced as activity increases, much like in active particles. The simulation data are in agreement with a theoretically constructed Rouse model of active polymer, demonstrating that irrespective of the strength of activity, the long-time dynamics of the polymer chain is characterized by a universal Rouse-like scaling $D_{\text{eff}} \sim N^{-1}$, where N is the chain length. We argue that the presence of hydrodynamic interactions will only have an insignificant effect on the observed scaling behavior.

CPP 19.10 Tue 12:15 H47

A Pulsating Active Solid — •Umang A Dattani[1], Francesco Serafin[1], Jonas Ranft[2], and Etienne Fodor[1] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg City, Luxembourg — [2]Institut de Biologie de l ENS, Ecole Normale Superieure, CNRS

Active matter has garnered significant attention in recent decades due to its numerous parallels with biological systems. Inspired by recent studies of biological tissues, such as cardiac cells, where constituent cell sizes periodically vary, a new form of activity termed ”pulsating active matter” has been introduced recently. We propose a model of a pulsating active solid, consisting of size-changing particles linked by a triangular spring network. Despite the fixed connectivity, our model exhibits a variety of patterns and topological phase defects, akin to previous studies. Additionally, we explore the elastic continuum limit, which successfully predicts several essential features of the microscopic model. We conclude by highlighting intriguing properties of this system and its different potential parallels.

Invited Talk CPP 19.11 Tue 12:30 H47

Emergent correlations and boundary fluctuations in epithelial cell sheets — •Silke Henkes — Lorentz Institute, Leiden University, Leiden, The Netherlands

In soft active materials, the driving motion of individual constituents competes with their mechanical interactions, giving rise to active liquids, solids or glasses. An especially important example of this are epithelial cell sheets, which form a barrier function in the body and where the active crawling motion of cells over the substrate acts against cell-cell adhesion and repulsion.

I will show that a minimal model of cell sheets with uncorrelated activity, based on active Brownian dynamics and a vertex model, is a good quantitative match to data from two experiments on corneal and MDCK cell sheets. Its core feature is an emergent correlation length, arising from the diffusive spread of active forces through an elastic solid. This is a very general result that emerges in many active solids.

The boundary of such cell sheets exhibits a ’fingering instability’ where the initially straight boundary develops large, spatiotemporally correlated fluctuations. Despite previous interpretations within many frameworks as an instability, I will show that it can be fully explained as arising from the active correlations of the cell sheets driving the boundary.

CPP 20: Interfaces and Thin Films I

Time: Tuesday 11:30–13:00 Location: H38

Invited Talk CPP 20.1 Tue 11:30 H38

Tailored polymer thin films enabled by initiated chemical vapor deposition (iCVD): From fundamentals to functional applications — •Stefan Schröder — Christian-Albrechts-Universität zu Kiel, Kiel, Germany

Functional polymer thin films are of great interest in vast application fields ranging from electronic devices to biomedical interfaces. Device miniaturization and the consequent need for new polymer films on the nanoscale demand precise thickness control and defect free films. Solvent-free initiated chemical vapor deposition (iCVD) meets these demands, because it circumvents de-wetting and surface tension effects encountered in conventional solution-based polymer thin film fabrication. The process provides conformal polymer coatings on the nanoscale on large-area substrates as well as complex geometries. In addition, it enables deposition on delicate substrates like flexible organic substrates, copy paper and biomedical patches at room temperature. This talk demonstrates the versatility of the iCVD process and highlights recent results from fundamental studies based on density functional theory (DFT) on the underlying reaction processes up to the application of iCVD films in sensors, biomedicine and electronic devices.

CPP 20.2 Tue 12:00 H38

Highly Electrically Conductive PEDOT:PSS films via Layer-by-Layer Electrostatic Self-Assembly — •Muhammad Khurram, Sven Neuber, Annekatrin Sill, and Christiane A. Helm — muhammad.khurram@uni-greifswald.de

Electrically conductive films of Poly(3,4-ethylenedioxythiophene): poly(styrenesulfonic acid) (PEDOT:PSS) are usually formed by spin coating of aqueous dispersions with PEDOT:PSS nanoparticles. The adsorption conditions are investigated using dip coating and a flow cell with different flow rates. Multilayer films are formed by sequential adsorption of oppositely charged macromolecules. PEDOT:PSS serves as polyanion, and PDADMA is the polycation. In dip coating, the first layer consists of approximately 70 nm thick monolayer of PEDOT:PSS nanoparticles. Subsequent PDADMA/PEDOT:PSS bilayers have a low, constant thickness (9.5 nm). Using the flow cell (0.2 mL/min) for film preparation also resulted in a constant PDADMA/PEDOT:PSS bilayer thickness (7.5 nm). PEDOT:PSS nanoparticle monolayers could also be observed with the flow cell, but only if the washing step after PEDOT:PSS adsorption was omitted. The films prepared by flow cell showed the highest conductivity (230 kS/m) and the lowest roughness (2 - 4 nm). We propose that the adsorption in a flow cell leads to a nearly flat orientation of the PEDOT molecules, increasing charge carriers' mobility. We also find that the relative humidity strongly influences the volume density and mobility of the charge carriers

CPP 20.3 Tue 12:15 H38

DFT Study of Catalyst-Ionomer Interactions in Hydrogen Fuel Cells — •Johanna Weidelt[1], Fabian Tipp[1], Tobias Binninger[1], and Michael Eikerling[1,2] — [1]Theory and Computation of Energy Materials (IET-3), Institute of Energy Technologies, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Chair of Theory and Computation of Energy Materials, Faculty of Georesources and Materials Engineering, RWTH Aachen University, 52062 Aachen, Germany

Proton exchange membrane fuel cells (PEMFCs) are promising devices for electricity generation from hydrogen. High efficiencies at low temperatures are achieved with platinum (Pt) as catalyst and Nafion as ionomer material. Because of the environmental persistence of the perfluorinated Nafion chains, fluorine-free ionomer materials are searched that maintain PEMFC performance and durability. To this end, the influence of the ionomer on the catalysis of the oxygen reduction reaction (ORR) in the cathode catalyst layer must be considered. Previous studies suggested that interactions between ionomer and Pt surface can compete with the adsorption of oxygenated ORR intermediates and negatively affect the catalytic activity. In this talk, we present a computational study investigating the competitive adsorption of ionomer species and reaction intermediates at a Pt(111) surface using grand-canonical density functional theory simulations. The Pt-adsorbate interaction strength was evaluated and surface phase diagrams were derived from adsorption energies calculated in implicit water environment under constant electrode potential.

CPP 20.4 Tue 12:30 H38

Dynamical and morphological changes of polyethylenimine thin films in relation to its CO2 absorption performance — •Maximilian Brückner[1], Martin Tress[1], Soma Ahmadi[2], and Shiwang Cheng[2] — [1]Peter Debye Institute for Soft Matter Research, Physics Department, Leipzig University, Germany — [2]Department of Chemical Engineering and Materials Science, Michigan State University, United States

Chemical reactions between carbon dioxide (CO2) and amine have been extensively characterized, however, their influence on the dynamics of polyamines remains largely unexplored. In this work, we compare the dynamics of polyethylenimine (PEI) before and after CO2 absorption through broadband dielectric spectroscopy (BDS). The molecular processes of bulk PEI are very different from those of thin film PEI, highlighting an interesting interface and nano-confinement effect. Detailed analyses show CO2 absorption slows down the PEI dynamics, which is consistent with an elevated glass transition temperature of PEI upon CO2 absorption. Further aspects of thin-film-preparation, namely the impact of molecular weight, film thickness, used solvent and plasma treatment of the substrate on surface roughness were investigated by atomic force microscopy and reveal pronounced de-wetting which did not occur in high-molecular-weight PEI on plasma-treated surfaces. The observed changes in dynamics and morphology are likely to reduce the performance of large-scale CO2 capture devices based on low-molecular weight PEI in porous silica, thus suggesting modifications of this approach.

CPP 20.5 Tue 12:45 H38

Thermo-Responsive Surface Structure and Wetting of Polymer Brushes with Octadecyl Side Chains — •Billura Shakhayeva[1], Franziska Neuhaus[1], Luciana Buonaiuto[2], Sander Reuvekamp[2], Sissi de Beer[2], Frieder Mugele[2], and Björn Braunschweig[1] — [1]University of Münster, Institute of Physical Chemistry, Münster (Germany) — [2]University of Twente, Physics of Complex Fluids, Enschede (The Netherlands)

Polymers are extensively studied as coatings due to their ability to respond to environmental changes, such as temperature or humidity variations, which greatly influence their wettability. This study investigates the effect of temperature on the molecular structure of poly-octadecylmethylacrylate (P18MA) brushes and their wetting behavior with hexadecane. Vibrational sum-frequency generation (SFG) spectroscopy was used to examine the molecular structure at the brush surface, both in air and in contact with hexadecane, by recording in situ SFG spectra near the three-phase contact line. The SFG spectra showed strong CH stretching bands of the octadecyl side chains at the air interface, indicating partial chain ordering that varies with temperature. For brushes in air, a phase transition at 311 K was identified as the surface melting temperature, 3 K higher than the bulk melting point. In the presence of hexadecane, surface melting occurred at 309 K, likely due to liquid penetration. Optical microscopy also revealed halo formation around the drop, suggesting local brush swelling. Below the surface melting point, the contact angle gradually decreased, while crossing the melting point enhanced hexadecane spreading.

CPP 21: Modeling and Simulation of Soft Matter II

Time: Tuesday 14:00–15:30 Location: H34

CPP 21.1 Tue 14:00 H34

Hard anisotropic particles: Excluded volume and second virial coefficients in arbitrary dimensions of space — •Markus Kulossa and Joachim Wagner — University of Rostock, Rostock, Germany

Precondition for investigations of phase behavior and equation-of-state data of many-particle systems are closed expressions for their free energy. The virial series gives access to the compressibility factor and therewith to the excess free energy of real supercritical fluids formed by hard, anisometric particles. Using Parson's approach, in many cases expressions solely based on the second virial coefficient accounting for the initial departure from ideal-gas behavior are used. In this contribution, we provide analytical expressions for the excluded volume of hard convex particles in arbitrary-dimensional Euclidean spaces. In addition to the detailed influence of the geometry and aspect ratio, we investigate the influence of singularities in the surface curvature. Analytical expressions for the excluded volume and second virial coefficients are of crucial importance for numerical calculation of higher-order virial coefficients. We provide so far unknown expressions for geometrical measures of uniaxial solids of revolution such as hyperellipsoids, hyperspherocylinders, hypercylinders, and hyperdoublecones in higher-dimensional Euclidean spaces.

CPP 21.2 Tue 14:15 H34

Navigating Chemical Space: An Active Learning Strategy Using Multi-Level Coarse-Graining — •Luis Walter and Tristan Bereau — ITP, Heidelberg University

Exploring the vast chemical compound space remains a significant challenge due to the immense number of possible molecules and limited scalability of conventional screening methods. To approach chemical space exploration more effectively, we have developed an active learning-based method that uses transferable coarse-grained models to compress chemical space into varying levels of resolution. By using multiple representations of chemical space with different coarse-graining resolutions, we balance combinatorial complexity and chemical detail. To identify target compounds, we first use an autoencoder to transform the discrete molecular spaces into continuous latent spaces. We then perform Bayesian optimization within these latent spaces, using molecular dynamics simulations to calculate target free energies of the coarse-grained compounds. This multi-level approach allows for an effective balance between exploration at lower and exploitation at higher resolutions. We demonstrate the effectiveness of our method by optimizing molecules to enhance phase separation in phospholipid bilayers. Our funnel-like strategy not only suggests optimal compounds, but also provides insight into relevant neighborhoods in chemical space. We show how this neighborhood information from lower resolutions can be used to guide the optimization at higher resolutions, thereby providing an efficient way to navigate large chemical spaces for free energy-based molecular optimization.

CPP 21.3 Tue 14:30 H34

Tuning Pore Size in Integral-Asymmetric, Isoporous Membranes via Bidisperse Diblock Copolymers — •Jiayu Xie and Marcus Müller — Institute for Theoretical Physics, Georg August University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Integral-asymmetric isoporous membranes, widely used in water filtration, are fabricated using a combination of evaporation-induced self-assembly (EISA) and nonsolvent-induced phase separation (NIPS). Membranes must have pores of an optimal size; small enough to block target substances but not so small as to cause excessive water resistance. While pore size can technically be adjusted by varying the copolymer's degree of polymerization, this approach requires synthesizing new copolymers for each desired pore size. A more economical alternative is blending polymers, where tuning the blending ratio of different components offers a feasible way to control pore size. However, mixing different copolymers could lead to macrophase separation. In this study, we focus on bidisperse diblock copolymers, and employ self-consistent field theory and particle-based simulations to explore the range of pore sizes over which this blending strategy is effective in fabricating membranes. Specifically, we aim to (1) establish correlations between system parameters and pore size and (2) elucidate the effects of these parameters on the dynamic behavior during SNIPS and the resulting membrane morphologies. Our findings provide valuable insights for the cost-effective fabrication of filtration membranes with tailored pore sizes.

CPP 21.4 Tue 14:45 H34

Machine-Learning potentials to understand pairing and stacking at the origin of life — •Laurie Stevens[1], Riccardo Martina[2], Alberta Ferrarini[2], and Marialore Sulpizi[1] — [1]Faculty of Physics and Astronomy, Ruhr-Universität Bochum, Germany — [2]Chemical Science Department, Università degli Studi di Padova, Italy

When exploring the origin of life, one main question remains open: how did we get from single nucleotides to long RNA and DNA chains which then led to more complex biological structures, following the RNA world hypothesis. More specifically, we are interested in how the nucleotides interactions are able to promote the synthesis of long polynucleotides. Experimental studies suggest that free nucleotides in water spontaneously organize into small molecular columnar phases, promoting the ligation of nucleic acid chains. To uncover the mechanisms behind this self-assembly, we use Molecular Dynamics simulations combined with Machine-Learning approaches.

Ab initio methods are too computationally expensive for the timescale of interest and for the complexity of the investigated systems. To overcome this limitation, we use Neural Network Potentials (NNPs) trained with DeepMD-kit and reinforced by metadynamics. After mastering the static and dynamical properties of a single Adenosine Monophosphate (AMP) in water, we are now investigating the stacking and pairing interactions between several AMPs by predicting the free energy landscape of this system as a function of the relevant degrees of freedom.

CPP 21.5 Tue 15:00 H34

Influence of hydroxyl groups on the dielectric constant of polyethylene — •Roshal Perepadan Shaju[1], Guido Roma[1], and Xavier Colin[2] — [1]Université Paris-Saclay, CEA, Service de recherche en Corrosion et Comportement des Matériaux, SRMP, Gif sur Yvette, 91191, France — [2]PIMM, Arts et Métiers Institute of Technology, CNRS, CNAM, HESAM University, 151 Boulevard de L'Hôpital, 75013 Paris, France

Polyethylene (PE) is widely used as an insulation for electric cables in various environments, including nuclear power plants. PE is susceptible to chemical modifications when exposed to ionizing radiation and oxidative environments. Introducing polar functional groups to this semi-crystalline PE, such as carbonyls and hydroxyl (OH) groups, has been observed to modify its dielectric response. However, the precise influence of hydroxylation on the dielectric properties of semi-crystalline PE is still inadequately understood. In this paper, we employ DFT and Density Functional Perturbation Theory (DFPT) to systematically investigate the effect of OH groups on the dielectric properties of semi-crystalline PE. By modeling PE with distinct surface, amorphous, and crystalline regions, the complexity of its semi-crystalline nature is explored. The static and high-frequency dielectric constants of polyethylene systems with different concentrations of OH groups were determined. The orientation of the OH defect relative to various crystallographic axes is thoroughly examined in order to determine how the alignment of the defects in the crystal lattice may affect the dielectric tensor.

CPP 21.6 Tue 15:15 H34

Load-induced shear band formation in microscale epoxy materials — •Julian Konrad, Janina Mittelhaus, Bodo Fiedler, and Robert Meissner — Hamburg University of Technology

Thin epoxy films (≈ 30 μm) exhibit unexpected ductile behavior under mechanical load, challenging the conventional view of thermoset materials as inherently brittle. This behavior is characterized by the formation of shear bands, as revealed by mechanical testing and infrared spectroscopy. Analysis of vibrational spectra shows redshifts in *para*-phenylene stretching vibrations due to bond elongation, and blueshifts in out-of-plane hydrogen vibrations, resulting from polarization effects in the aromatic backbone. Molecular dynamics simulations support these findings, revealing a cascade of molecular realignments driven by deformation. Notably, these structural changes are reversible upon heating, suggesting a form of frozen entropy elasticity rather than plasticity. To further investigate, we employed a novel method using the MACE neural network potential to compute vibrational spectra with *ab initio* accuracy. This approach captures strain-dependent spectral shifts, accounts for interface and size effects, and highlights key implications for the design of composite materials.

CPP 22: Organic Electronics and Photovoltaics II

Time: Tuesday 14:00–15:15 Location: H38

CPP 22.1 Tue 14:00 H38

Spontaneous orientation polarization in mixed films of organic semiconductors — •Albin Cakaj, Alexander Hofmann, and Wolfgang Brütting — Experimental Physics IV, Institute of Physics; University of Augsburg, 86135 Augsburg, Germany

Small organic molecules processed by physical vapor deposition (PVD) can exhibit a preferential alignment, despite their tendency to form glassy amorphous films. This alignment can additionally lead to a macroscopic polarization of the film, if the molecules have a permanent dipole moment (PDM). The additional field, also referred to as giant surface potential (GSP), can impact the properties of organic light emitting diodes (OLEDs) significantly. Therefore, understanding the formation and control of this effect is of crucial importance.

We investigated different GSP forming polar molecules mixed with non-polar organic compounds. We found combinations with enhanced PDM alignment, where the impact of suppressed dipole-dipole interactions by dilution is far more significant than the effect on the film-formation process by a change in the effective glass temperature of the blend. Additionally, our data hint to the conclusion that molecules with an already high degree of PDM alignment keep their magnitude of alignment in mixed films without significant enhancement. Therefore, we can conclude that mixing of polar molecules with a non-polar compound can enhance the degree of PDM alignment significantly, if the polar molecules exhibit only a small degree of PDM alignment in the first place.

CPP 22.2 Tue 14:15 H38

Ultrafast Response in Unbalanced Mobility Organic Photodetectors — •Felix Hergenhan, Tianyi Zhang, Karl Leo, and Johannes Benduhn — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, TU Dresden, Dresden, 01187 Germany

Organic photodetectors (OPDs) have attracted growing interest due to their potential in various optoelectronic applications. However, the slower response speed of OPDs compared to their inorganic counterparts, primarily influenced by low charge carrier mobilities, has hindered their application in high-speed technologies. In this presentation, we will discuss the dynamic behavior of OPDs, focusing on how ultrafast response times can still be achieved despite significant mobility imbalance and overall low mobility. Importantly, the role of RC (resistance-capacitance) limitations is emphasized, as they significantly impact the achievable response speed of the devices. We systematically investigated the effects of device design, device dimensions, light intensity, and applied bias on OPD performance and its dynamic behavior. Notably, special features could be identified in their dynamic response that led to improved rise and fall times of only a few nanoseconds and a cutoff frequency beyond 10 MHz. We propose a model explaining the origin of these features and demonstrate how to utilize them to achieve faster response times. By exploring the entire picture of device design, material choice, and operational conditions, we provide an outlook on the future development of ultrafast OPDs.

CPP 22.3 Tue 14:30 H38

Systematic variation of acceptor and donor moieties in donor-accerptor-donor small molecules for efficient room-temperature phosphorescence — •Uliana Tsiko, 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

Room-temperature phosphorescence (RTP) from purely organic materials promises unique application in diverse fields including molecular sensing, bioimaging, information storage, and anti-counterfeiting. With the design of programmable luminescent tags (PLTs), we recently reported a novel photonic device architecture that is well suited for various labelling and information exchange applications and even allows a biodegradable design. However, improved RTP emitters are required to fully exploit this technology.

In our contribution, we systematically analyze the impact of the acceptor and donor moieties on the photophysical properties of newly synthesized RTP emitters to gain an understanding of structure-property relationships. While the electron-accepting character does not significantly affect the emission properties, the electron-donating ability of the donor unit can strongly improve RTP emission, leading to pronounced sky-blue phosphorescence in purely organic materials, which has been rarely observed before. These emitters are further characterized in PLTs as a prototypical excitonic application scenario.

CPP 22.4 Tue 14:45 H38

Efficient room-temperature phosphorescence in small-molecule hosts for applications in information storage — •Yana Bui Thi, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden

Room-temperature phosphorescence (RTP) from organic materials promises unique applications in molecular sensing, bioimaging, and information storage. Typically, RTP is achieved by embedding emitter molecules in a rigid matrix to suppress non-radiative decay. The integration of such emitters into polymer hosts has enabled advancements in photonic technologies, such as programmable luminescent tags. However, a comprehensive understanding of host-guest interactions, particularly with small-molecule hosts suitable for vacuum processing, is widely missing. This work investigates the photophysical properties of RTP emitters embedded in wide bandgap small molecules, typically used in OLEDs. Thin films are fabricated either by spin coating or thermal evaporation, the latter offering superior film quality and compatibility with patterning techniques. RTP can be promoted or impaired depending on the choice of the host material, partially even allowing for RTP in the presence of oxygen. A significant enhancement of photoluminescence can be obtained due to favorable energy transfer from host to emitter. These results highlight the importance of the host selection in optimizing emitter performance and present valuable insights for polymer-free RTP-based photonic devices.

CPP 22.5 Tue 15:00 H38

Regulated Growth of Benzoperylene-TCNQ Charge-Transfer Complex Crystalline Networks — •Kirill Gubanov, Yana Reva, Stevie Furxhiu, Fabian Streller, Yifan Bo, Phillip Greissel, Dirk M. Guldi, and Rainer H. Fink — Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

Highly ordered luminescent organic micro- and nano-crystals of charge-transfer complexes (CTC) are generating a considerable interest due to their prospective applications in miniaturized and multifunctional optoelectronics. We propose a strategy of controlled crystallization growth of Benzoperylene (BP)-TCNQ-CTC nanorods network. As a result of the distinct polarity-based solubility of BP and TCNQ, 2D microsheets of BP of tunable sizes can be used as templates for the CTC nanorod meshes growth in solution. The optical and electronic properties of the respective CTC were additionally investigated. Emission spectroscopy revealed a significant quenching of the BP strong fluorescence upon CTC formation: electron excitation in BP leads to a charge transfer to a non-emissive TCNQ and to non-radiative relaxation. Using NEXAFS micro-spectroscopy, we examined the electronic structure and a temperature-dependent band gap modification. Thus, collective insights into the BP-TCNQ CTC properties provide valuable information for material optimization for future applications in optoelectronic devices. The research is funded by the BMBF (contract 05K19WE2) and SolTech initiative.

CPP 23: Polymer and Molecular Dynamics, Friction and Rheology

Time: Wednesday 9:30–11:15 Location: H34

Invited Talk CPP 23.1 Wed 9:30 H34

Advanced combined rheometer setups to in-situ correlate molecular dynamics and molecular structure formation with mechanical properties — •Manfred Wilhelm — Karlsruhe Institut für Technologie, Karlsruhe, Germany

Molecular understanding of mechanical properties over a broad length and time scale is crucial to develop advanced materials. Our research aims to design and built unique combined rheometer setups that can monitor in-situ molecular observables, such as molecular dynamics or chemical functional groups that are directly correlated to the macroscopic mechanical responses. These combined experimental setups overcome the experimental challenges associated with offline measurements and facilitate the understanding of structure-property relationships.

CPP 23.2 Wed 10:00 H34

Nonequilibrium Dynamics of the Helix-Coil Transition in Polyalanine — •Maximilian Conradi[1], Henrik Christiansen[1,2], Suman Majumder[3], Fabio Müller[1], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany — [2]NEC Laboratories Europe GmbH, Kurfürsten-Anlage 36, 69115 Heidelberg, Germany — [3]Amity Institute of Applied Sciences, Amity University Uttar Pradesh, Noida 201313, India

In this work, the nonequilibrium pathways of the collapse of the helix-forming biopolymer polyalanine are investigated. To this end, the full time evolution of the helix-coil transition is simulated using molecular dynamics simulations. At the start of the transition short 310-helices form, leading to the molecule becoming more rod-like midway through the collapse. Afterwards, α-helix formation becomes the prevalent ordering mechanism leading to multi-leg hairpin structures, representative for the equilibrium behavior of longer chains. The dynamics of this transition is explored in terms of the power-law scaling of various associated relaxation times as a function of the chain length.

CPP 23.3 Wed 10:15 H34

Porous Particles Formation in the Drying of Polymer Solution Droplets — •Mengmeng Wu, Hsiao-Ping Hsu, and Kurt Kremer — Max-Planck-Institut für Polymerforschung, Mainz, 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 formation of drying polymer solution droplets. By maintaining below the glass transition temperature, highly porous particles are generated followed by a fast evaporation and cavitation of solvents. For a drying droplet in an environment with low thermal conductivity, the temperature experiences a decrease owing to solvent vaporization. Such temperature reduction results in a decrease in evaporation rate 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 23.4 Wed 10:30 H34

Polymer chains under oscillatory force in solvents of variable quality — •Bogumiła Szostak[1,2], Ron Dockhorn[2], Jens-Uwe Sommer[2], and Jarosław Paturej[1,2] — [1]University of Silesia in Katowice, Bankowa 12, 40-007 Katowice, Poland — [2]Leibniz Institute of Polymer Research Dresden, Hohe Straße 6 D-01069 Dresden, Germany

Polymers are key materials in soft condensed matter with diverse applications. Recently, significant attention has been given to understanding the micromechanical behavior of single macromolecules under applied forces. Using molecular dynamics, we examined how constant and periodic forces affect polymer chain conformations in dilute solutions, modeled for good and poor solvents. We systematically calculated the projection of the end-to-end vector in the force direction as a function of the applied force. This analysis led to the construction of force-extension diagrams, which revealed conformational transitions of polymers from a globular state to an extended chain. Analysis of hysteresis loops for periodic forces showed that longer force periods allowed more time for the system to respond, resulting conformational reorganization. These results were compared with analytical solutions of the Rouse model under periodic perturbation and scaling laws, providing a valuable benchmark and deeper insight into the observed dynamics. We also characterized the relationship between dissipated energy and the frequency of the applied sinusoidal stretching force. These findings provide new insights into the mechanical behavior of polymer chains under oscillatory forces, enhancing our understanding of their dynamic properties and potential applications.

CPP 23.5 Wed 10:45 H34

Role of Trapped Water Molecules at Sliding Contacts in Lattice-Resolved Friction Investigated with Molecular Dynamics — •Miljan Dašić and Igor Stanković — Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

Understanding nanoscale friction within an environment which contains water, is crucial for engineering friction-based mechanisms and characterizing surfaces. From the point of view of Friction Force Microscopy (FFM) experiments, it has been understood that the lattice resolution in water environments originates from a dry contact state, in case of which all water molecules get expelled from the gap between the microscope's tip and the studied substrate.

We have developed an All-Atom Molecular Dynamics simulation setup, for revisiting this understanding by performing a detailed analysis of the impact of water molecules present in the system on the dynamic behavior of the nanotribological contact between an amorphous SiO2 probe and a monolayer MoS2 substrate.

Our analysis of stick-slip patterns shows the entrapment of water molecules at the contact interface. These trapped water molecules act as an integral part of the probe and participate in its interaction with the substrate, hence affecting the probe's dynamics and preventing long slips. Surrounding water molecules from the capillary or layer of water exhibit a replenishing effect, acting as a water reservoir during the sliding process. Such a phenomenon enables the preservation of lattice-scale resolution across a range of normal loads.

CPP 23.6 Wed 11:00 H34

The analytical investigation of star polymers in confined geometries — •Zoriana Danel[1], Joanna Halun[2], and Maciej Dudek[3] — [1]Cracow University of Technology — [2]Institute of Nuclear Physics — [3]Academy WSB

The analysis of the influence of star polymer topology on the depletion interaction potentials, the depletion forces and Pincus force was carried out analytically. The method of calculation of the dimensionless depletion interaction potentials and the dimensionless depletion forces for a dilute solution of ideal star polymers with f=3, 4, 5 legs in a Θ - solvent confined in a slit geometry of two parallel walls with repulsive surfaces and for the case of one repulsive and the other inert surface was proposed. Besides, we performed the investigation of the elastic properties of star polymers with different number of legs in a semi-infinite space confined by single wall with different boundary conditions and calculated Pincus force in the above mentioned cases. Calculations were carried out for star polymers with f=3,4,5 legs attached to the substrate by one or two arms. The acquired results showed that the Pincus force is affected by the number of arms attached to the surface. The obtained results are interesting from scientific and industrial point of view, because of their potential use in the production of paints, varnishes and new functional materials. Star polymers, due to their topology and shape can find practical application in nano - technology, as well as in biotechnology and medicine for drug and gene transmission.

CPP 24: Hybrid and Perovskite Photovoltaics III

Time: Wednesday 9:30–11:15 Location: H38

CPP 24.1 Wed 9:30 H38

Tailored perovskite crystallization by passivation molecule engineering for efficient light-emitting diodes — •Jungui Zhou[1,2], Min Zhu[1], Yufeng Zhai[2], Shouzheng Chen[2,4,5], Benedikt Sochor[2], Sarathlal Koyiloth Vayalil[2], Lei Cai[3], Man-Keung Fung[1,6], Peter Müller-Buschbaum[5], and Stephan V. Roth[2,7] — [1]Soochow University, Suzhou, China — [2]DESY, Hamburg, Germany — [3]Shandong normal university, Shandong, China — [4]FRM II, Garching, Germany — [5]TUM School of Natural Sciences, Garching, Germany — [6]MUST, Macau, China — [7]KTH Royal Institute of Technology, Stockholm, Sweden

Metal halide perovskite light-emitting diodes (PeLEDs) are regarded as alternative candidates for next-generation display technologies.Various additives have been widely used in perovskite precursor solutions, aiming to improve the as-obtained perovskite film quality through passivating defects and controlling the crystallinity. Although the defect passivation of additives has been intensively investigated, a deep understanding of how additives influence the crystallization process of perovskites during the spin-coating and annealing processes is still lacking. Here, by combining In-situ photoluminescence (PL) and grazing-incidence wide/small-angle X-ray scattering (GIWAXS/GISAXS) techniques, a systematic study of the perovskite film-formation process, perovskite structure, and inner morphology of CsPbBr3 perovskite films modified by various additives is conducted, revealing the influence of additives on the formation of high-quality perovskite films and efficient PeLEDs.

CPP 24.2 Wed 9:45 H38

Optical In-Situ Methods as Process Optimization Toolbox — •Lennart Reb — Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109, Berlin

In the field of perovskite photovoltaics, precursor optimization is often guided by the visual inspection of film quality by experienced researchers. However, combined optical in-situ techniques can help shift toward rational, evidence-based process design. In-situ characterization methods are frequently used for studying the reaction kinetics during processing: Optical techniques to monitor solvent evaporation, such as spectral absorption, reveal changes in halidoplumbate spectral signatures that correlate with the increasing density of polynuclear plumbate species. Photoluminescence (PL) measurements further elucidate early perovskite nucleation during quenching processes and crystal growth. Structural insights from grazing-incidence X-ray scattering (GIWAXS) track intermediate phases, the formation of perovskite structures, and the evolution of secondary phases. This work briefly reviews the state-of-the-art multimodal in-situ characterization techniques and introduces the multimodal μ slot-die coater, a small-scale platform integrating UV-vis, PL, imaging, and GIWAXS capabilities. Initial results of combined measurements demonstrate its power for studying perovskite film formation during scalable processing, offering insights into reaction kinetics and showcasing the capabilities of in-situ imaging techniques in scalable perovskite deposition. For example, in-situ PL measurements show the changes of PL signal over time upon the inclusion of chloride-based additives.

CPP 24.3 Wed 10:00 H38

Metal halide perovskite solar cells under space like temperature conditions — •Simon Alexander Wegener[1], Altantulga Buyan-Arivjikh[1], Kun Sun[1], Zerui Li[1], Xiongzhuo Jiang[1], Matthias Schwarzkopf[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany

Perovskite solar cells hold great promise for space applications due to their exceptional properties, including high power-to-weight ratios and efficiencies comparable to silicon cells. Their solution processability lowers both manufacturing and launch costs, presenting a cost-effective alternative to gallium arsenide cells. However, their viability in space is challenged by harsh conditions such as high vacuum, extreme temperatures, and radiation. This study investigates the impact of extreme temperature fluctuations in low Earth orbit, ranging from -100*C to +100*C, on perovskite solar cell performance. Operando GIWAXS measurements enable real-time analysis of the crystal structure under simultaneous illumination and thermal cycling. Measurements of I-V curves and optical absorption spectra further assess electrical and optical properties. Results reveal temperature-dependent efficiency variations and degradation influenced more by device layers and interfaces than the active layer itself. Understanding the mechanical, optical, and electrical behavior of the entire cell assembly under such conditions is key to optimizing durability and performance.

CPP 24.4 Wed 10:15 H38

Simulation of the impact of processing conditions for solution-processed thick perovskite layers — •Martin Majewski[1], Shudi Qiu[2], Larry Lüer[2], Vincent M. Le Corre[2], Tian Du[2], Olivier J.J. Ronsin[1], Christoph J. Brabec[2], Hans-Joachim Egelhaaf[2], and Jens Hartin[1] — [1]Helmholtz Institue Erlange-Nuernberg, Cauerstraße 1, 91058 Erlangen, Germany — [2]Institute of Materials for Electronics and Energy Technology (i-MEET), Friedrich-Alexander Universitaet Erlangen Nuernberg

Fabricating thick (1000 nm) solution-processed perovskite layers is expected to increase the efficiency of carbon-contact-based solar cells compared to thinner (500 nm) films. However, increasing only the deposited layer thickness often results in buried voids inside the dry film. Recently, we have developed a theoretical framework based on Phase Field simulations. With the help of the simulations, it is possible to explain why voids form in the film. The crystals nucleate at random spots inside the liquid film. The movement of the condensed-vapor interface, due to evaporation, leads to an agglomeration of the crystals at the film surface. The crystals block further evaporation and the remaining solvent is the origin of the buried voids inside the dry film. We explain how adding seeds on the substrate before coating the thick film can prevent this. In this case, processing conditions have to be modified compared to standard operating procedures for thin films. The theoretical expectations can be verified experimentally, leading to a performance improvement of the devices.

CPP 24.5 Wed 10:30 H38

First-principles modelling of hybrid perovskites — •Udo Schwingenschlögl and Aleksandra Oranskaia — King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

The photoconversion efficiency record of silicon-perovskite solar cells exceeds 30% owing to hybrid perovskites with organic cations that stabilize the perovskite by non-covalent bonding. To address the electronic properties and stability issue from the perspectives of the bulk crystal phases, point defects, and surfaces and interfaces (requiring large simulation cells) the computational methods must be chosen carefully: (1) For the structural relaxation an exchange-correlation functional is required that adequately describes materials rich in $\mathrm{NH}\cdots\mathrm{I}$ bonding (between organic cations and I) and $\mathrm{I}\cdots\mathrm{I}$ bonding (between PbI_6 octahedra or between PbI_6 octahedra and I-related defects). (2) For the electronic structure calculation an exchange-correlation functional is required that adequately describes the spin-orbit coupling of the Pb and I electrons. Comparing the PBE, PBE-TS, PBE-D3, PBEsol, vdW-DF2, and rVV10 functionals for relaxing FAI, $C_4N_2H_{12}(I_3)_2$, $C_6H_7NI(I_3)$, I_2, In, $Cs(I_3)$, $Cs_2(I_3)_2(I_2)$, and PbI_2 crystals, we show that the rVV10 functional provides the most balanced prediction for the types of non-covalent bonding relevant for hybrid perovskites. We also discuss problems related to the HSE06 functional and show that the PBE functional with a Hubbard correction for the Pb 6p and I 5p orbitals (together with fully relativistic pseudopotentials) provides promising results.

CPP 24.6 Wed 10:45 H38

An effective Population balance model for evaporation-driven precursor-mediated crystallization — •Kai Segadlo, Olivier Ronsin, and Jens Harting — Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IET-2), Erlangen, Germany

Although tremendous progress has been made in recent years in Experimental and Material Design for solution-processed photoactive Perovskite thin films, this progress has not likewise been followed by a corresponding improvement in the theoretical understanding of these systems. In particular, the high computational demands arising from the plethora of potentially relevant thermodynamic processes, such as evaporation, crystallization, chemical reactions, demixing, and advection, as well as the high costs of in situ multichannel screening experiments, lead to uncertainties about the underlying physical mechanisms, which in practice often facilitate the use of narrow empirical models. As a first step towards theoretical coherence, we combine empirical mass transport models into a single population balance model accounting for evaporation, crystallization, and chemical reactions. We validate the drying subpart against drying curves, and the crystallization subpart against crystallinity curves from Ultraviolet Imaging Spectroscopy, and Phase field simulations, respectively. The model allows us to gauge the relevances of the processes during precursor-mediated methylammonium lead iodide crystallization measured with in situ Grazing Incidence Wide Angle X-ray scattering and to shed light on the experimentally highly relevant but hard-to-access coupling between evaporation and crystallization.

CPP 24.7 Wed 11:00 H38

Modeling and Analysis of Spectral and Thermal Effects in 2-Terminal Perovskite-CIGSe Tandem Solar Cell Configurations — •Yokozuna Schirmer[1], Nicolas Otto[1], Guillermo Farias Basulto[2], Rutger Schlatmann[1,2], Bert Stegemann[1], and Christof Schultz[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

Tandem solar cells are being developed to exceed the efficiency limits of single-junction cells. Typically, they are designed in a 2-terminal (2T) current-matched configuration, which can result in a reduced energy yield due to current mismatch caused by spectral variations throughout the day. To overcome this limitation, tandem solar cells can be configured in a 2T voltage-matched setup, which could mitigate the impact of spectral sensitivity on performance. The aim of this work is the development of a computational model to analyse the energy yield of each configuration. This model combines temperature-dependent electrical cell parameters with spectrally resolved real-world outdoor data to simulate the operational behaviour and to evaluate the advantages of each interconnection approach. The model is validated by measured I-V cell data from single- and multi-junction cells. Moreover, a comprehensive analysis of the calculated results provides valuable insights into the performance trade-offs under real-world conditions, enabling the identification of the optimum design for specific applications.

CPP 25: Poster: Active Matter, Soft Matter, Fluids (joint session DY/CPP)

Time: Wednesday 10:00–12:00 Location: P3

CPP 25.1 Wed 10:00 P3

Enhanced stability and chaotic condensates in multi-species non-reciprocal mixtures — •Laya Parkavousi[1], Navdeep Rana[1], Ramin Golestanian[1,2], and Suropriya Saha[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), D-37077 Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

Random non-reciprocal interactions between a large number of conserved densities are shown to enhance the stability of the system towards pattern formation. The enhanced stability is an exact result when the number of species approaches infinity and is confirmed numerically by simulations of the multi-species non-reciprocal Cahn-Hilliard model. Furthermore, the diversity in dynamical patterns increases with increasing number of components and novel steady states such as pulsating or spatiotemporally chaotic condensates are observed. Our results may help to unravel the mechanisms by which living systems self-organise via metabolism.

CPP 25.2 Wed 10:00 P3

Non-reciprocal Model B and the role of mobilities and non-reciprocal interfacial forces — •Bibhut Sahoo[1] and Peter Sollich[1,2] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen — [2]Department of Mathematics, King's College London, London

Recently the effects of non-reciprocal interactions have been widely studied in the Cahn-Hilliard model for phase separation, which is based on a magnetic analogy. Here we explore the corresponding nonreciprocal model B, as the continuum theory for non-reciprocal particle mixture. We focus on the effect of mobility matrix on topology of the phase diagram and find that changing mobility can change stability of a homogeneous state, which for reciprocal interactions would be impossible. We study spinodal dynamics in regions of instability, where static or travelling spinodal patterns can occur. This aspect is as in non-reciprocal Cahn-Hilliard but, the transitions between these instabilities are novel: they occur not via exceptional points, but via first order transitions in the length scale of the dominant unstable modes. At transition, a static and a travelling spinodal pattern with two different scales coexist. We show that more complicated transitions involving coexistence of three length scales can also occur. We finally argue, based on a nonreciprocal version of Dean's equation, that coarse graining into a model B description should lead to non-reciprocal interface terms, rather than only in the bulk as assumed in theories to date. We show that such interfacial terms can significantly enlarge the travelling spinodal regions in the phase diagram.

CPP 25.3 Wed 10:00 P3

Mixed active fluids of two kinds — •Astik Haldar — Universität des Saarlandes, Saarbrücken 66123, Germany

We explore here the polar active fluids of two types, characterizing by their different aligning and propulsion strengths. We example here the fluids as the collections of moving living creatures, which could fuel itself through chemical reactions in their body . We called this system as active system, and consider their brilliant interactions. We here try to model those through considering some parameters and physically observable quantities. We find the parameters region where they have their oriented flocking as parallel or antiparallel, ordered rotating phase coherently meaning chiral phase. Our study finds the transition between the phases as saddle node as well as pitchfork bifurcation in mean field theory scheme. We find different kind of pattern formed states appear through the analytical as well as numerical study.

CPP 25.4 Wed 10:00 P3

Verification, efficiency analysis and extension of the kinetic Event-Chain Algorithm — •Nico Schaffrath, Tobias Kampmann, and Jan Kierfeld — TU Dortmund, Dortmund, Germany

The novel cluster kinetic Monte-Carlo algorithm, which is based on the event-chain Monte-Carlo method, is specifically designed to simulate systems of two-dimensional self-propelled hard particles. We verify this algorithm from scratch by analysing various single-, two- and many-body systems, as well as some algorithm-specific quantities. To gain insight about the applicability of the algorithm, we compare its performance to that of an Event-Driven Brownian-Dynamics simulation. Finally, we investigate the possibility to simulate particles with soft interaction energies as well as an extension to three-dimensional systems. Regarding the latter, the phase diagram of self-propelled hard spheres is calculated.

CPP 25.5 Wed 10:00 P3

AMEP: Analyzing Active Matter Simulations in Python — Kay-Robert Dormann[1], Lukas Hecht[1], Kai Luca Spanheimer[2], Aritra K. Mukhopadhyay[1], Mahdieh Ebrahimi[1], Suvendu Mandal[1], and •Benno Liebchen[1] — [1]Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Darmstadt, Germany — [2]Institut für Theoretische Physik II, Heinrich-Heine-Universität, Düsseldorf, Germany

The **A**ctive **M**atter **E**valuation **P**ackage (AMEP)[1] is an easy-to-use Python library for analysing simulation data of particle-based and continuum simulations. It provides a powerful interface for handling complex analysis of large data sets from different simulation software such as LAMMPS, HOOMD-blue, GROMACS and others. A plethora of methods to calculate observables and visualise results make AMEP suitable to calculate complex observables not only for beginners but also for advanced studies of active and soft matter. AMEP is written in pure Python and leverages powerful and well-known libraries such as NumPy, SciPy and Matplotlib. Computationally expensive methods are parallelized to run on laptops and workstations as well as high-performance computing clusters.

The methods range from order parameters, cluster methods, spatial and time correlation functions to thermodynamic properties and coarse-graining methods. More information and examples are available at https://amepproject.de. AMEP can be installed via conda and pip.

[1] L. Hecht et al., arXiv:2404.16533 [cond-mat.soft]

CPP 25.6 Wed 10:00 P3

Fluctuation induced network patterns in spatially correlated noise — •Sebastian Fehlinger[1], Kai Cui[2], Arooj Sajjad[1], Heinz Koeppl[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, Institut für Physik Kondensierter Materie, Hochschulstraße 8, 64289 Darmstadt — [2]Technische Universität Darmstadt, Selbstorganisierende Systeme, Merkstraße 25, 64283 Darmstadt

Fluctuations play an important role in many fields of physics, from quantum electrodynamics to statistical mechanics. In active matter physics, so far, most works have focused on active particles that are subject to thermal fluctuations caused by the surrounding solvent. Here, we explore the collective behaviour of active particles under the influence of spatially correlated noise, that can arise, e.g., from fluctuating external fields. Therefore, we introduce a minimal model which describes the dynamics of (chiral) active particles with alignment interactions in a time-dependent Gaussian random field, that features a characteristic spatial correlation length, but no temporal correlations. Using Brownian dynamics simulations, we find, that the active particles aggregate to system spanning, percolated networks. These structures are (i) fluctuation-induced, (ii) feature local alignment of the contained particles, but no global alignment, and (iii) hardly show any coarsening. We systematically characterize the emerging patterns with tools from topological data analysis (persistence diagrams, Vietoris-Rips complexes and Betty numbers).

CPP 25.7 Wed 10:00 P3

Reconfiguring hydrodynamic flow fields of active particles by light — Lisa Rohde, Tom-Hannes Hemann, Gordei Anchutkin, and •Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, University Leipzig, Leipzig, Germany

Microscopic active particles propel themselves via localized energy conversion, generating hydrodynamic flow fields that govern their boundary interactions and collective behaviour. The long-range behaviour of the flow patterns classifies them as either pushers, which expel fluid along their swimming axis, or pullers, which draw fluid inward. In nature, some microorganisms can adaptively switch between pusher and puller modes in response to their environment. However, synthetic active particles are currently limited to a fixed pusher or puller configuration during fabrication, constraining our ability to study their dynamic responses to environmental cues. Here, we present a self-thermophoretic active particle that can reconfigure its flow field on demand during the experiment. This is achieved by illuminating the particle with an inhomogeneous light field shaped by a spatial light modulator. The illumination patterns create surface temperature fields inducing thermo-osmotic flow fields that propel the particle and shape the hydrodynamic interactions. By using gold nanoparticles, we trace and characterize the hydrodynamic flow field of the active particle. The ability to dynamically alter the propulsion characteristics will enable us to investigate and control their interactions and collective dynamics.

CPP 25.8 Wed 10:00 P3

Brainbots as smart autonomous active particles with programmable motion — •Isa Mammadli[1], Martial Noirhomme[2], Nathan Vanesse[2], Jayant Pande[3], Ana-Sunčana Smith[1], and Nicolas Vandewalle[2] — [1]PULS, Institute for Theoretical Physics, FAU Erlangen-Nürnberg, 91058, Erlangen, Germany — [2]GRASP, Institute of Physics B5a, University of Liege, B4000 Liege, Belgium — [3]Department of Physical and Natural Sciences, FLAME University, Pune, India

We introduce an innovative robotic device designed to enable controlled motion for the study of active matter. Motion is driven by an internal vibrator, powered by a compact rechargeable battery. The system integrates acoustic and magnetic sensors alongside a programmable microcontroller. Unlike conventional vibrobots, this device employs a motor that generates horizontal vibrations, producing cycloidal trajectories that have been thoroughly characterized and optimized. Specific segments of these trajectories can be harnessed to create tailored motion patterns. As a proof of concept, we demonstrate how this versatile system can be used to develop active particles exhibiting diverse dynamics, ranging from ballistic motion to run-and-tumble diffusive behavior. Based on experimental data, we provide a simulation routine capable of replicating these trajectories, enabling the generation of extended datasets and the exploration of various input velocity configurations. This approach facilitates the determination and prescription of optimized input parameters for applications such as enhanced search strategies and precise path following.

CPP 25.9 Wed 10:00 P3

Fundamental Measure Theory for active hard discs — •Jonas Buba and Michael Schmiedeberg — Theoretical Physics: Lab for Emergent Phenomena, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The behavior of active soft particles has been studied extensively and provides a good model for many active matter systems [1]. However, some systems might be described more accurately by considering hard particles instead. While active soft particles have been described with a Phase Field Crystal approach (e.g., in [2]), a similar description of active hard particles is still lacking. In our approach we use Fundamental Measure Theory [3] to model hard discs and add activity. We expect to gain further insight into the role that the particle type can play in dynamical pattern formation.

[1] Marchetti M C, Joanny J F, Ramaswamy S, Liverpool T B, Prost J, Rao M and Simha R A. Hydrodynamics of soft active matter. Rev. Mod. Phys. 85 1143, 2013. [2] Arold D and Schmiedeberg M. Mean field approach of dynamical pattern formation in underdamped active matter with short-ranged alignment and distant anti-alignment interactions. J. Phys.: Condens. Matter 32 315403, 2020. [3] Roth R, Mecke K, and Oettel M. Communication: Fundamental measure theory for hard disks: Fluid and solid. The Journal of Chemical Physics, 136(8):081101, 2012.

CPP 25.10 Wed 10:00 P3

Many-Body Dynamics of actively rolling fibers — •Alex Arnhold[1], Falko Ziebert[1,2], and Igor M Kulic[3,4] — [1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, 69120 Heidelberg, Germany — [2]BioQuant, Heidelberg University, Im Neuenheimer Feld 267, 69120 Heidelberg, Germany — [3]Institut Charles Sadron UPR22-CNRS, 67034 Strasbourg, France — [4]Institute Theory of Polymers, Leibniz-Institute of Polymer Research, D-01069 Dresden, Germany

Fiberboids are active filaments, capable of self-propulsion, whose dynamics were recently described in [A. Bazir, A. Baumann, F. Ziebert, I. M. Kulić, Soft Matter 2020]. So far, only single and simple 2-body dynamics of fiberboids were described.

In this work we will take a first look at the many-body dynamics. Specifically, we analyze a system of multiple nylon-rods, which when heated from below display self-propelled rolling motion. Confining the rods to roll on a single axis only, implements a simple realization of an 1D active gas. We analyze the experiments concerning clustering and nonequilibrium fluctuations and rationalize the system by simple lattice models.

CPP 25.11 Wed 10:00 P3

Pumping currents and formation of flocks in 1D Ising model — •Adrian Morais Cabral and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Germany

Non equilibrium systems create phenomena that are not observed in equilibrium counterparts, such as long range order in two or less dimensions and breaking of detailed balance.

We use an effective description of coupled Langevin equations to study a 1D system where an Ising order parameter is coupled to a charge density. Our assumption is that the charge current has a contribution proportional to the order parameter for the driven system. The formation of domain walls leads to a source of dynamical frustration for the charge. Driving disallows the formation of domain walls and creates flocking blob like states in addition to constant ordered and disordered states and a non moving spike phase. These solutions are studied numerically in 1D for $T \geq 0$.

At $T = 0$, we characterize existing flocking solutions and compare analytical predictions to numerical simulations which agree well with only one fitting parameter.

At finite temperatures we find new dynamics for the flocking state such as reversals similar to the active Ising model and (quasi) crossings. However, we have not yet been able to answer whether the existing ordered phase is stable in 1D.

CPP 25.12 Wed 10:00 P3

Statistical Field Theory for Vicsek-type models — •Carsten

Littek, Falko Ziebert, and Matthias Bartelmann — Institut für Theoretische Physik, Universität Heidelberg, Germany

Dry, aligning, dilute active matter systems display a wide range of emergent phenomena such as collective, orientationally ordered motion and phase separation. The self-propelled particles in such systems undergo noisy aligning interactions with their neighbours, but they do not exchange momentum with their surrounding. While microscopic and hydrodynamic descriptions, whose connection involves approximations, exist, their predicted behaviour - such as scaling exponents - do not match.

Here we present a microscopic statistical field theory for active Brownian particles inspired by Mazenko (2010). In our formulation we interpret the particles' two-dimensional positions and their direction of motion as Martin-Siggia-Rose (MSR) fields to obtain a path integral representation of the N-particle partition function. The MSR action is augmented by a two-particle interaction that aligns particle directions either ferromagnetically as in the Vicsek model or nematically. Similar to quantum many-body theory the benefit of our field theoretic formulation of Vicsek-type models is that it allows for developing a self-consistent perturbation theory and using renormalization techniques. Our aim is the calculation of density and velocity correlation functions in the homogeneous ordered phase and the transition into the ordered phase.

CPP 25.13 Wed 10:00 P3

Coupling reaction-diffusion and locomotion in vegetative cells — •Blaž Ivšić[1], Piotr Nowakowski[2], Igor Weber[2], and Ana Sunčana Smith[3,2] — [1]Institut za fiziku, Zagreb, Croatia — [2]Institut Ruđer Bošković, Zagreb, Croatia — [3]Friedrich-Alexander- Universität, Erlangen, Germany

Cellular locomotion involves the dynamic interplay between signaling molecules, cytoskeletal activity, and membrane deformation. We present a computational model coupling protein Rac1 reactiondiffusion dynamics to cell locomotion to study vegetative state of amoeba Dictyostelium discoideum. Rac1 regulates actin polymerization via effectors like WASP and Arp2/3, while GAP modulates its activity. The model captures Rac1 dynamics on a deforming membrane, reproducing experimentally observed spatiotemporal patterns.

Cell shape is modeled using a Level-set method to track membrane dynamics, driven by forces linked to Rac1 concentration. Specifically, surface tension and normal forces (due to interaction of the cell with the substrate) proportional to Rac1 concentration influence membrane movement. The dynamics are conveyed through a fluid velocity field obtained by solving a time-dependent Stokes equation.

Our model replicates Rac1 activity patterns seen in live-cell imaging and links these patterns to cell motility. By bridging Rac1 reactiondiffusion dynamics with membrane mechanics, the model provides insights into the mechanisms of actin-driven locomotion in vegetative cells.

CPP 25.14 Wed 10:00 P3

Numerical Simulation of Microplastic Permeation in Soil: from Solutes to Particles — •Hao Liu[1], Yifan Lu[2], Christina Bogner[2], Martin Lörder[1], and Stephan Gekle[1] — [1]University of Bayreuth, Bayreuth, Germany — [2]University of Cologne, Cologne, Germany

Microplastics have become significant environmental pollutants, raising concerns about their accumulation and distribution across ecosystems. Although terrestrial environments, particularly soils, often exhibit high levels of microplastic contamination, they remain relatively understudied. Microplastic transport in soil involves complex interactions among particle properties, soil structure, and fluid dynamics. Understanding mechanisms such as permeation, aggregation, and degradation is essential for effective environmental risk assessments and strategies to control microplastic pollution.

This study aims to simulate and predict soil hydraulic conductivity in microplastic-laden flows. Challenges include modeling behaviors of microplastic particles as they transport in soil with complex porous structures. High-resolution μCT scans of soil samples will provide the necessary porous media data, and simulations will be conducted using FluidX3D software. The research progresses in two phases: first, disregarding particle size and shape to analyze solute transport mechanisms; second, incorporating detailed particle properties to study transport and accumulation in pores. The goal is to model microplastic dynamics for accurate predictions of microplastic distribution in soil systems.

CPP 25.15 Wed 10:00 P3

Thermo-Osmotic Flows via Anti-Stokes Cooling — •akshay kallikkunnath[1], kamil bruchal[2], pawel karpinski[2], and frank cichos[1] — [1]Molecular Nanophotonics, Peter Debye Institute for Soft Matter Physics, Faculty of Physics and Earth System Sciences, Leipzig University, Germany — [2]Faculty of Chemistry, Institute of Advanced Materials, Wroclaw University of Science and Technology, Poland

Fluidic manipulation has gained huge interest over time especially with the studies on metal nanoparticles as optically controlled heat sources generating temperature gradients. With recent developments in the synthesis of lanthanide doped crystals which can be cooled by anti-stokes cooling, we try to bring laser cooling of microcrystals to the field of fluidics. In this work, we optically trap and cool ytterbium doped NaYF4 crystals by means of anti-stokes cooling. Temperature measurements for such microscale cooled crystals are done using a technique which utilizes the phase transition of liquid crystals. With such a thermal gradient created using cold sinks in liquid, we study and provide for the first time experimental and numerical results for flows generated at solid-liquid boundary, i.e., thermo-osmotic flows. The results will provide further scope for studying dipolar thermo-osmotic and corresponding thermo-electric fields in an electrolyte solution generated by arranging optically heated and cooled particles together. Our findings can have direct implications on the study of temperature-dependent biochemical processes which inhibit with lower temperature or on response of a biological specimen to low temperature stress or may even find application in local cryotherapy.

CPP 25.16 Wed 10:00 P3

Thermodynamically consistent coarsening model of crossover placement in meiosis — •Marcel Ernst[1,2] and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Universität Göttingen, Germany

Crossovers play an important role in meiosis, ensuring correct segregation of homologous chromosomes and increasing genetic variability. A recently proposed model suggests that crossover placement is determined by biomolecular condensates that coarsen by exchange and diffusion of a protein along chromosomes, consistent with experiments. We here present an extended model including exchange with the nucleoplasm based on thermodynamic principles. We study theoretically and numerically the initial protein loading onto the chromosome, the droplet growth regime, the coarsening regime, and the final equilibrium. We derive scaling laws for the number of crossovers analogous to Lifshitz-Slyozov-Wagner theory in different limits. Finally, we investigate the effect of protein exchange with the nucleoplasm on crossover placement and compare the results with empirical data from several species. In conclusion, our model allows us to explain key features of meiotic crossover placement in wild type and several mutants.

CPP 25.17 Wed 10:00 P3

A lattice Boltzmann approach to electrolytic multiphase flows — •Alexander Reinauer and Christian Holm — Institute for Computational Physics, Stuttgart, Germany

Simulating electrolytic multiphase flow presents significant challenges, often requiring either the detailed modeling of large numbers of particles or solving complex, nonlinear partial differential equations, such as the Navier-Stokes and Nernst-Planck equations. While particle-based simulations provide molecular details, continuum-scale approaches, including the Navier-Stokes and Nernst-Planck equations, enable the study of larger systems relevant to applications in oil recovery, biological processes, and waste treatment.

In this work, we extend the Lattice Boltzmann Method using a Color-Gradient approach to simulate immiscible two-phase flow, coupled with a custom Nernst-Planck solver for the transport of dissolved charged species. This coupling allows to incorporate the preferential solubilities of chemical species.

Our implementation, based on the pystencils/lbmpy framework, generates highly optimized code for both CPU and GPU architectures. To validate the model, we performed simulations of freely suspended liquid droplets subjected to an external electric field. Additionally, we explored contact angle models and initiated studies on applying the approach to porous media under varying conditions.

CPP 25.18 Wed 10:00 P3

Coarsening of chemically active droplets — •Stefan Köstler[1,2], Yicheng Qiang[1], and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]University of Göttingen, Institute for the Dynamics of Complex Systems, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Droplets formed by phase separation play an important role in cellular organization and are widely used in the design of synthetic cells and lab-on-chip devices. Droplet emulsions typically coarsen due to surface tension and hydrodynamic effects, which generally prevents precise control over droplet sizes. While coarsening can be suppressed by active chemical reactions, it is unclear how these reactions affect the coarsening dynamics and control droplet sizes. To elucidate this, we numerically simulate a binary mixture that phase separates and undergoes reactions. We find three different dynamical regimes: Small droplets are dominated by coalescence due to hydrodynamic advection, then transition to an Ostwald ripening regime dominated by diffusion, and finally exhibit size control by active chemical reactions. We predict the transition from ripening to size control analytically, and we validate our analytical estimate of the final size using a numerical minimization of a surrogate equilibrium free energy. Our theory provides an improved understanding of coarsening mechanisms, allowing to achieve greater control of emulsions.

CPP 25.19 Wed 10:00 P3

Zetapotential of Gold Surfaces in a Flow Cell — •Mattis Rasenat, Peter Vogel, Marcus Witt, and Thomas Palberg — Johannes gutenberg Universität Mainz

We present a case study on the zeta-potential of gold surfaces in a continuous flow cell. The charge of dielectric surfaces is of high interest for technological applications. Therefore, we measure the zeta potential of polymer particles in a custom-made electrokinetic flowthrough cell with exchangeable sidewall. The zeta potential is measured with a super-heterodyne light scattering setup.

CPP 25.20 Wed 10:00 P3

Use of molecular CO_2 for surface charge regulation — Peter Vogel[1], Markus U. Witt[1], David Beyer[2], Christian Holm[2], Muhammad Navaz Qaisrani[3], Marialore Sulpizi[4], and •Thomas Palberg[1] — [1]Inst. of Physics, JGU, Mainz, Germany — [2]Inst. of Computational Physics (ICP), U Stuttgart, Stuttgart, Germany — [3]MPI for Polymer Research, Mainz, Germany — [4]Dept. of Physics, RU Bochum, Bochum, Germany

In deionized water CO_2 forms carbonic acid which partially dissociates. Such 'realistic' salt free systems contain a significant background electrolyte concentration and a pH of 5.5. Both lowers the effective charge of dielectric surfaces. Surprisingly, the remaining molecular CO_2 causes an additional drastic decharging effect, even to complete decharging in water equilibrated against pure CO_2. Molecular CO_2 acts directly on the degree of dissociation and thus lowers the bare charge, while effective charges merely follow suit. MD simulations show the formation of a diffusely adsorbed monolayer of CO_2, which locally lowers the dielectric constant. Based on this we suggested dielectric charge regulation as novel decharging mechanism. If then salts are added to the carbonized surfaces, one finds recharging by co-ion adsorption. This process is favoured by hydrophobicity, by co-ion size and, most important, also by the amount of adsorbed CO_2. Given the ubiquity of dielectric surfaces in contact with aqueous electrolytes, this very general charge regulation processes appear to be of great fundamental and practical importance.

CPP 26: Nanostructures, Nanostructuring and Nanosized Soft Matter I

Time: Wednesday 11:30–13:00 Location: H34

Invited Talk CPP 26.1 Wed 11:30 H34

Polyelectrolytes in the confined space of mesopores for transport regulation — •Annette Andrieu-Brunsen — Technische Universität Darmstadt, Macromolecular Chemistry - Smart Membranes, Germany

Nanopores are a key component in various technologies from oil production, separation and sensing, to drug delivery or catalysis and energy conversion. In contrast to technological pores, biological pores and channels demonstrate highly precise transport being directed, highly selective, and gated. A key factor to this performance is their nanoscale structure, and their local control on charge regulation and polarity in confined space. Inspired by this performance and precision we are interested in understanding the relation between the design of polymers in nanoscale space and its resulting properties to for example understand and advance transport performance of technological pores.

This talk will give insights into the interplay of polymer functionalization of mesoporous layers and resulting ionic mesopore accessibility. Among others, the effect of increasing polyelectrolyte amount and thus increasing charge density as well as the influence of polymer chain composition and the observation of confinement-induced pKa shifts will be discussed. Furthermore, ionic transport regulation by gradually adjusting the wettability of mesopores will be demonstrated including the influence of nanoscale wettability step-gradients in mesoporous silica layers. To indicate next steps our activities towards increasing precision in polymer functionalization of mesoporous silica materials will be outlined.

CPP 26.2 Wed 12:00 H34

Infrared Scanning Near-Field Spectroscopic Insights into Self-Assembled Block Copolymer Nanostructures — •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 — [2]IMSEAM — [3]BioQuant, Heidelberg University, Germany

Block copolymers (BCPs) are known for their ability to self-assemble into a variety of morphologies on the nanometer scale. While the self-assembly of 2D thin films has been extensively investigated, less attention has been paid to 3D bulk morphologies. In this work, the internal nanostructure of long-range ordered 3D bulk morphologies of a well-defined diblock copolymer consisting of polystyrene and a methacrylate-based copolymer is studied by means of infrared scanning near-field optical microscopy (IR-SNOM). We demonstrate that by irradiation at an absorption band specific to one polymer block, it is possible to chemically image the blocks nano-ordered spatial arrangement [1]. Representative images were successfully correlated with scanning electron microscopy (SEM) data. By altering the molar fraction of polymer blocks, a variety of nanostructures was imaged. For some polymer compositions, the nanostructure formed was observed to change upon post-functionalization. Additionally, nanotomography of the bulk material is approached by imaging and volume reconstruction of serial sections.

[1] B. Weidinger, N. von Coelln et al., Polym. Chem., **15** (2024) 4093-4100.

CPP 26.3 Wed 12:15 H34

Star-like molecular brushes with poly(2-oxazoline)-based amphiphilic diblock copolymer side arms — •Wenqi Xu[1], Laura Fietzke[2], Rustam A. Gumerov[3], Feifei Zheng[1], Peiran Zhang[1], Cy M. Jeffries[4], Dmytro Soloviov[4], 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, Dresden, Germany — [3]DWI Leibniz Institute for Interactive Materials, RWTH Aachen University, Aachen, Germany — [4]EMBL at DESY, Hamburg, Germany

Poly(2-oxazoline)s (POx) are synthetic, non-toxic, and biocompatible polymers developed to replace the increasingly immunogenic poly(ethylene glycol) in biomedicine. Among many architectural variants of POx, studies on POx-based star brushes are still scarce. In the present work, we investigate molecular brushes, in which diblock copolymers from hydrophilic poly(2-methyl-2-oxazoline) and hydrophobic poly(2-*n*-butyl-2-oxazoline) are grafted onto star-shaped poly(methyl methacrylate) backbones with the stars having functionalities ranging from 2 to 5. The size and shape of the star brushes were investigated in dilute aqueous solutions using computer simulation, dynamic light scattering, and synchrotron small-angle X-ray scattering. Our results show that these star brushes form ellipsoids with different degrees of elongation. Moreover, a size growth is found for the star brushes at high temperatures, which is attributed to the aggregation of the amphiphilic side arms.

CPP 26.4 Wed 12:30 H34

STED-inspired optical lithography beyond acrylates —

Sourav Islam, Georgii Gvindzhiliia, and •Thomas A. Klar — Institut für Angewandte Physik, Johannes Kepler Universität Linz, Austria

STED-inspired[1], and hence sub-diffractional, nanolithography was so far restricted to free radical polymerizations, predominantly of (meth)acrylates.[2] We now expand the STED-inspired toolkit to cationic[3, 4] and oxidative polymerizations,[5] comprising the technologically important classes of epoxides and pi-conjugated polymers. In both cases, we achieved structure sizes below 100 nm using transient-state absorption depletion (TAD) in systems comprising depletable photosensitizers, optionally combined with onium salts. The pi-conjugated nanostructures are particularly intriguing, because they potentially will allow for sub-diffractional organic electronic devices.

[1] Klar, Hell, Opt. Lett. 24, 954 (1999). [2] Fischer, Wegener, Las. Phot. Rev. 7, 22 (2013). [3] Islam, et al., J. Phys. Chem. C 127, 1873 (2023). [4] Islam, Klar, ACS Omega 9, 19203 (2024). [5] Islam, et al., Proc. SPIE 1299503(2024).

CPP 26.5 Wed 12:45 H34

In-situ investigation of the lateral and vertical structure of PNIPAM-microgels at the air-liquid and solid-liquid interfaces — Olaf Soltwedel, Joanne Zimmer, •Hayden Robertson, and Regine von Klitzing — Institut für Physik Kondensierter Materie, Technische Universität Darmstadt, D-64289 Darmstadt, Germany

The novel surface characterisation approaches presented here highlight, for the first time, the use of both specular and off-specular X-ray reflectivity (XRR) to probe the vertical and lateral structure of adsorbed polymer microgels particles at various interfaces, offering *in situ*, non-invasive insights without the need for doping or transfer-induced artefacts. In particular, we demonstrate the complementarity of two readily accessible laboratory techniques on characterising the structure of adsorbed microgels: atomic force microscopy (AFM) and XRR. Initial *ex situ* AFM scans of Langmuir-Blodgett deposited microgels at the solid interface revealed strong lateral 2D hexagonal ordering across a broad range of surface pressures. However, for the first time, these results are confirmed by off-specular XRR, demonstrating the existence of the hexagonal long-range ordering at low and intermediate surface pressures for *in situ* conditions at the air-water interface. Upon uniaxial compression of the interface, the microgel lattice constants decrease monotonically, indicating tighter packing. At these higher surface pressures, both AFM and off-specular XRR also reveal the formation of microgel domains; hexagonal short-range ordering is maintained whereas long-range ordering is diminished.

CPP 27: Molecular Electronics and Excited State Properties II

Time: Wednesday 11:30–13:00 Location: H38

CPP 27.1 Wed 11:30 H38

Break-junctions beyond single-molecule conductance — •Joseph Hamill — Department of Chemistry and Nanoscience Center, University of Copenhagen, Denmark

The challenge in nanosciences is to reliably manipulate and probe objects on the atomic and molecular scale. Single-molecule break junctions cleverly integrate a single molecule into an electric circuit, enabling measurement of its thermal, electrochemical, and electrical properties. These studies explore candidates for waste heat capture, quantum information technologies, sensors, nanomedicine, and other novel materials applications. Over the past 20 years, single-molecule break junction methods have advanced to measure current, resistance, rectification, and thermopower. Despite this progress, they are not yet a staple in every chemist's toolbox like NMR spectroscopy. Recent studies using these junctions to monitor and induce chemical reactions may change this. I will present two recent studies demonstrating their sensitivity to changes in bonding chemistry and the tautomer state of single molecules in the junction. This sensitivity is unlocked through frequency domain spectroscopy using flicker noise analysis[1] and improved machine learning approaches, such as principal component analysis and k-means clustering.[2]

[1] U. Rashid, W. Bro-Jørgensen, K. Harilal, P. Sreelakshmi, R. R. Mondal, V. Chittari Pisharam, K. N. Parida, K. Geetharani, J. M. Hamill, and V. Kaliginedi. JACS, 146, 9063-9073. [2] P. Sreelakshmi, R. Mahashaya, S. Leitherer, U. Rashid, J. M. Hamill, M. Nair, P. Rajamalli, and V. Kaliginedi. JACS, 10.1021/jacs.4c12423.

CPP 27.2 Wed 11:45 H38

Charge transport in organic semiconductors with a mapping approach to surface hopping — •Johan Runeson[1], Thomas Drayton[2], and David Manolopoulos[2] — [1]Institute of Physics, University of Freiburg, Germany — [2]Physical and Theoretical Chemistry Laboratory, University of Oxford, UK

Coupled charge-phonon systems are challenging to simulate in the intermediate regime between traditional delocalized band theory and localized polaron theory. In particular, it remains unclear which methods are suitable to describe organic semiconductors. Conventional trajectory-based methods, such as Ehrenfest dynamics and surface hopping, do not capture the correct equilibrium of mixed quantum-classical systems. In this talk, I will present a simple solution to this problem. Based on a recently developed "mapping approach to surface hopping" [1,2], we propagate trajectories on the adiabatic state with the highest population, which in contrast to previous methods is consistent with the correct quantum-classical equilibrium. We applied this methodology to charge diffusion in crystalline rubrene [3] and obtained a well-defined diffusion constant, without having to introduce the phenomenological relaxation time approximation (RTA). Our results give 30-60 % higher charge mobilities than conventional RTA calculations and shed light on experiments of the optical conductivity.

[1] J. R. Mannouch and J. O. Richardson, J. Chem. Phys. 158, 104111 (2023). [2] J. E. Runeson and D. E. Manolopoulos, J. Chem. Phys. 159, 094115 (2023). [3] J. E. Runeson, T. J. G. Drayton, and D. E. Manolopoulos, J. Chem. Phys. 161, 144102 (2024).

CPP 27.3 Wed 12:00 H38

Influence of Classical Molecular Motion on Energy Transport in Molecular Aggregates — •Ritesh Pant[1], Sebastian Wüster[2], and Alexander Eisfeld[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Indian Institute of Science Education and Research, Bhopal, India

Molecular aggregates can transport electronic excitation energy over large distances due to dipole-dipole interactions [1]. We explore the impact of classical thermal motion of entire monomers on this transport, considering a chain of molecules [2]. Such motion induces changes in the aggregate's geometry, thereby altering the exciton states and enabling, in certain regimes, the adiabatic transport of excitation energy. We find that, in the absence of intramolecular vibrations, the interplay between molecular motion and exciton dynamics induces oscillatory behavior in site populations, which are coupled to the motion. These oscillations occur specifically when the molecular motion is slow enough to be considered adiabatic with respect to the exciton dynamics, and their characteristics depend on the chain length, with shorter chains exhibiting more pronounced effects. We also explore the effect of intramolecular vibrations on this oscillatory behavior and investigate the conditions under which the oscillations persist or are suppressed.
[1] T. Brixner et. al., Adv. Energy Mater. 7, 1700236 (2017).
[2] R. Pant et. al., Phys. Chem. Chem. Phys. 22, 21169 (2020).

CPP 27.4 Wed 12:15 H38

Enhancing excitonic properties in organic semiconductors by aqueous ions — •Filip Podjaski — Department of Chemistry and Centre for Processable Electronics, Imperial College London, UK

While organics semiconductors (OSC) promise tailorable structure-function relationships for enhanced solar energy conversion abilities, advancement is often hindered by limiting knowledge of interwoven photo-physical processes and properties that lead to recombination losses on ultrafast time scales.[1] Herein, I discuss possibilities to measure and modify functionalized OSC' exciton behaviour, to address their recombination. For photocatalysis, interactions with aqueous ions, which are also relevant for enabling sea water use, are typically disregarded. Our time-resolved optical spectroscopy study on suspended polymer nanoparticles in presence of different salts shows how they can improve stabilization of excitons. We further introduce Terahertz permittivity measurements as convenient tool to probe the complex permittivity / dielectric properties of OSCs on ps-time scales. The permittivity defines exciton binding energy and is hence relevant for charge carrier photogeneration and transport. But its highly frequency dependent values are commonly extracted orders magnitude off the ps-regime. Our study focussing on carbon nitrides now reveals dielectric screening and transport properties at the early time scales of solar energy conversion process chains, and illustrates environmental enhancements enabled by ions.[2]

References: [1] Nat. Rev. Mater. 6, 168-190 (2021). [2] R. Jahangir, F. Podjaski et al., submitted, arxiv.org/abs/2411.06226

CPP 27.5 Wed 12:30 H38

Computational insights into open-shell molecules for applications in molecular electronics — •Susanne Leitherer[1] and Gemma C. Solomon[1,2] — [1]Department of Chemistry and Center of Nanoscience, University of Copenhagen, Denmark — [2]Niels Bohr Institute, University of Copenhagen, Denmark

Recent studies have explored a range of molecules with unpaired electrons, represented by their spin. These investigations focused on the charge transport characteristics of the molecules when interfaced with electrodes, as well as their structural rearrangements in electric fields and interactions with surfaces. The theoretical analysis of these systems frequently employs spin-polarized or symmetry-broken unrestricted density functional theory (DFT). This method has proven effective in modeling oxidized molecules exhibiting highly conductive low-energy states, characterized as 1D topological insulators[1]. However, it is well known that DFT can pose challenges for open-shell structures due to their multiconfigurational nature. We demonstrate how for a selection of polycyclic aromatic hydrocarbons - previously investigated in recent scanning probe experiments[2] - the ground state can be accurately determined using a multi-configurational short-range DFT approach[3]. [1] High Molecular Conductance and Inverted Conductance Decay over 3nm in Aminium-Terminated Carbon-Bridged Oligophenylene-Vinylenes, Krieger et al, JACS (2024); [2] Atomically resolved single-molecule triplet quenching, Peng et al., Science 373 (2021); [3] Multiconfigurational sr-DFT for open-shell systems, Hedegard et al, J. Chem. Phys. 148, 214103 (2018)

CPP 27.6 Wed 12:45 H38

Exceptionally High Two-Photon Absorption Cross Sections in Quinoidal Diazaacene-Bithiophene Derivatives — •Gabriel Sauter[1], Antonia Papapostolou[2], Audrey Pollien[1], Kathleen Fuchs[3], Kerstin Brödner[3], Jan Freudenberg[3], Uwe H. F. Bunz[3], Andreas Dreuw[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut — [2]Interdisziplinäres Zentrum für Wissenschaftliches Rechnen — [3]Organisch-Chemisches Institut, Universität Heidelberg

In nonlinear optics, materials with high two-photon absorption (2PA) cross sections are crucial for bioimaging, photodynamic therapy, and 3D nanoprinting [1]. Our study highlights quinoidal diazaacene-bithiophene derivatives with exceptional 2PA cross sections, reaching 53,600 GM (850-950 nm) and 4,100 GM (1400-1600 nm), unmatched by organic chromophores of this size [3].

Using experimental z-scan techniques and TDDFT calculations, we attribute these properties to the chromophores acceptor-π-donor-π-acceptor structure, which ensures high oscillator strength and strong state coupling. These features optimize transition dipole moment alignment, maximizing 2PA efficiency.

These findings advance the development of efficient NIR-2PA materials for photonic and biomedical applications.

References:

1. F. Kröger et al., *RSC Appl. Polym.* **2024**, 2, 847.
2. K. Fuchs et al., *Angew. Chem. Int. Ed.* **2024**.

CPP 28: Modeling and Simulation of Soft Matter III

Time: Wednesday 15:00–16:00 Location: H34

CPP 28.1 Wed 15:00 H34

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

Bottom-up coarse-graining approaches frequently focus on reproducing structural order parameters, ensuring consistency with structural properties from the underlying atomistic model. However, these methods often struggle to predict thermodynamic quantities accurately, leading to challenges in transferability. Furthermore, the coarse-grained (CG) potential is typically highly sensitive to the mapping scheme, introducing representability issues. Recent CG models increasingly enhance traditional pair potentials by incorporating a potential that depends on the local density around each CG particle, which effectively includes many-body interactions in a mean-field approximation. We introduce local density dependent potentials based framework in the CG force-field for small conjugated molecules, which are widely used in the field of organic photovoltaic materials. Our framework captures the local density around each mapped CG site to ensure structural and thermodynamic accuracy, while enhancing computational efficiency compared to its atomistic counterparts.

CPP 28.2 Wed 15:15 H34

Simulation of the fabrication of integral asymmetric polymer membranes using continuum modeling — •Gregor Häfner and Marcus Müller — University of Göttingen, Germany

Integral asymmetric polymer membranes represent a promising class of functional macromolecular systems with a wide range of potential applications, including water purification and protein separation. Their synthesis is achieved through a two-step procedure: (i) the controlled self-assembly of diblock copolymers upon solvent evaporation, to form a cylindrical morphology that is oriented perpendicular to the solution-gas interface. (ii) a solvent-non-solvent exchange, raising the polymer concentration above its glass transition, thereby freezing the matrix phase while allowing the entry of the non-solvent through the cylindrical minority domains. Below, the non-solvent macrophase separates from the polymer to form a porous sub-structure.

In order to gain insight into the physical processes, we perform computer simulations. A continuum model is employed which treats the local concentrations as order parameters and minimizes a free-energy functional. In the limit of high viscosity, the dynamics are purely diffusive, enabling comparison with a particle-based model. We use the continuum model to optimize the final membrane morphology and identifying optimal parameter regions and dependencies. Additionally, this model enables the treatment of finite viscosities. We demonstrate that in the presence of a bariocentric flow, the frozen top layer can be transported downwards to prevent the formation of macro voids beneath the isoporous top layer.

CPP 28.3 Wed 15:30 H34

Highways in pore networks — •Werner Napetschnig[1], Ekaterina Baikova[1,2], Maximilian Fuchs[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

When simulating Stokes flow of gases through porous media, the volume flow is often explained by microstructural properties. However, most of these properties do not adequately account for the arrangement of pathways, which is strongly material dependent. Here, we highlight the importance of considering these pathways and explore different techniques to identify flow paths. A pore network model based on micro-computed tomography scans of paper samples serves as the basis for air flow simulation. Two methods are evaluated to identify transport pathways and locate the most critical flow regions. In the first method, the maximum flow rate between individual pores determines the paths. It is shown that the highest flow rate travels between fiber network layers and clusters at a few exit pores. The second method identifies paths iteratively through a stochastic approach where the flow rate is the weighting factor. We identified the most frequently used highway regions. In addition, we studied the orientation and geometric properties of these highways. Our results show that only a few segments within the highways significantly influence the overall flow. Therefore, these highways need to be numerically represented when defining the explanatory microstructure properties.

CPP 28.4 Wed 15:45 H34

A lattice Boltzmann study of bijels as a novel type of catalyst support structure — •Johannes Martinus Peter Beunen and Jens Harting — Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien, Cauerstraße 1, 91058 Erlangen, Germany

Due to their high surface area to volume ratio porous media are very suitable as catalyst support materials. However, the stochastic morphology of commercially available supports generally results in poor reaction product transport and inefficient use of the therein-contained catalyst material. These issues can be alleviated by making use of catalyst supports acquired from spinodally derived architectures due to their beneficial percolation properties. In particular, architectures obtained from bicontinuous interfacially jammed emulsion gels (bijels) seem to provide a viable route to manufacture stable catalyst supports that resolve the aforementioned issues. In this work, this type of porous support is further investigated by means of the three-dimensional lattice Boltzmann method. First, we simulate the formation of bijels by an extension of the lattice Boltzmann method, to allow for multicomponent fluids and particles with non-neutral wetting properties. We report on the improved properties of the resulting porous structures compared to stochastic equivalents for usage in chemical reactors. Hereafter, the lattice Boltzmann method is employed again to further validate the enhanced performance of bijel-derived geometries by means of reactive flow simulations. Our findings suggest that bijel-derived catalyst support structures allow for an almost threefold increase in reactor effectiveness.

CPP 29: Organic Electronics and Photovoltaics III

Time: Wednesday 15:00–16:00 Location: H38

CPP 29.1 Wed 15:00 H38

Energy band structure of image potential states of organic semiconductor on graphite studied by angle-resolved low-energy inverse photoelectron spectroscopy — •Tomoko Onishi[1] and Hiroyuki Yoshida[1,2] — [1]Chiba university, Chiba, Japan. — [2]Chiba university MCRC, Chiba, Japan.

The image potential state of the organic semiconductor molecule on the conductive surface is of particular interest because the image potential states can be sensitive probes of interfacial electronic states. Their energy band structure (the energy-momentum relation) provides detailed information about the electron behavior. Recently, we have developed the angle-resolved low-energy inverse photoelectron spectroscopy (AR-LEIPS) [1,2]. This technique allows direct observation of the unoccupied states without sample damage and with the resolution better than 0.3 eV. In this study, we applied AR-LEIPS to a monolayer of copper phthalocyanine (CuPc) on highly oriented pyrolytic graphite (HOPG). The observed band structure of the image potential state was parabolic, indicating that its nature is free-electron-like along the surface plane. By fitting the band structure to a quadratic function, we obtained the effective masses of the image potential states on HOPG and CuPc/HOPG to be (1.14 * 0.02) m0 and (1.33 * 0.08) m0, respectively, where m_0 is the electron mass. The effective mass becomes heavier due to the periodic potential induced by the CuPc molecule.[1] H. Sato, H. Ishii, H. Yoshida, et al., Nature Mat. 21, 916 (2022) [2] Y. Kashimoto, H. Yoshida et al, Rev. Sci. Instrum., 94, 063903 (2023).

CPP 29.2 Wed 15:15 H38

Fluorination of Thieno-quinoxalines enables tunable excitonic and electronic bandgaps — •Md Moidul Islam[1,2], Arthur Markus Anton[3], Shahidul Alam[4], Patrick Irmisch[3], Alexander J. Much[7], Ulrich S. Schubert[1,2], Christos Chochos[5,6], and Harald Hoppe[1,2] — [1]IOMC, FSU Jena, Humboldtstrasse 10, 07743 Jena, Germany — [2]CEEC Jena, Philosophenweg 7a, 07743 Jena, Germany — [3]Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Linnéstraße 5, D-04103 Leipzig — [4]KAUST Solar Center, PSE, MSE, Thuwal 23955-6900, Kingdom of Saudi Arabia — [5]Institute of Chemical Biology, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, Athens 11635, Greece — [6]Advent Technologies SA, Patras Science Park, Stadiou Street, Platani-Rio, 26504, Patra, Greece — [7]Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle, Germany

Thieno-quinoxaline conjugated polymers are an interesting class of organic semiconductors. While it is known that fluorination causes shifts in the molecular energy levels to deeper binding energies, the mechanisms behind are, so far, not well characterized. In this study, six thieno-quinoxaline polymers with a systematically increased number of fluorinated sites were investigated in solutions and films. Our results indicate a strong correlation between the extend of fluorination, the molecular planarity, and its ability to form aggregates. We also demonstrate, in unprecedented detail, how these structural properties influence various behaviors related to optical and electronic properties.

CPP 29.3 Wed 15:30 H38

Extending the design space of carbazole-based TADF emitters: From photophysical insights to OLED performance — •Karolis Leitonas[1], Łukasz Łapok[2], Sebastian Schellhammer[1], and Sebastian Reineke[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden — [2]Department of Physical Chemistry and Electrochemistry, Faculty of Chemistry, Jagiellonian University, Kraków, Poland

Although organic light-emitting diodes (OLEDs) dominate the market for mobile displays, e.g., in smartphones, designing efficient and long-lasting blue pixels remains challenging. Enhancing OLED efficiency requires effective singlet and triplet exciton harvesting - a key mechanism to minimize energy losses via non-radiative decay. Emitter materials exhibiting thermally activated delayed fluorescence (TADF) can achieve up to 100 % internal quantum efficiency (IQE) providing a promising approach for the design of efficient OLEDs. Still, their potential is not yet fully exploited due to incomplete insights into the underlying structure-property relationships and chemical design challenges. We discuss the photophysical properties of new emitters extending the class of carbazole-based TADF emitters introduced by Adachi et al. [1] and analyze their application in OLEDs.

[1] Uoyama et al. Nature 2012

CPP 29.4 Wed 15:45 H38

Predicting the molecular arrangement of organic optoelectronic materials — •Alexey Gudovannyy[1], Julia M. Schäfer[2], Olga Gerdes[2], Dirk Hildebrandt[2], Gunter Mattersteig[2], Martin Pfeiffer[2], and Frank Ortmann[1] — [1]Department of Chemistry, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany — [2]Heliatek GmbH, 01139 Dresden, Germany

The morphology of the most promising molecular semiconductor materials remains highly challenging to predict from scratch. If possible, it would still require a lot of computational time and sometimes experimental data. The main obstacle here is the exponential growth with the number of molecular degrees of freedom for bulky side groups, which forces one to search on extremely complex energy surfaces. However, organic semiconductors mostly exhibit a limited set of structural motifs, primarily herringbone and two-dimensional brickwork patterns. Constraining the search to such dimensionally reduced packing possibilities simplifies the process while preserving 3D structural features. Here, we present a cost-efficient workflow for predicting thermodynamically stable 2D arrangements of molecular periodic associates, where only the molecular structural formula is required. We theoretically and experimentally investigated a set of known and newly crystallized compounds of evaporable flexible molecules with interesting optoelectronic properties, predicted their packing in two-dimensional layers, and compared them with experimentally resolved crystal structures, obtaining a very good agreement in the packing.

CPP 30: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods I

Time: Wednesday 16:15–18:30 Location: H34

Invited Talk CPP 30.1 Wed 16:15 H34

Challenges and Opportunities in Bringing Machine Learning to a Synchrotron — •Alexander Hexemer[1], Tanny Chavez[1], Wiebke Köpp[1], Dylan McReynolds[1], Stephan Roth[2], Tim Snow[3], and Sharif Ahmed[3] — [1]Lawrence Berkeley National Lab, Berkeley, CA 94720 — [2]DESY, Hamburg, Germany — [3]Diamond Light Source, Didcot, UK

Artificial intelligence (AI) and machine learning (ML) are transforming scientific research, offering innovative solutions to longstanding data collection, analysis, and interpretation challenges. Synchrotron facilities, which generate vast amounts of complex, high-dimensional data, present unique opportunities to leverage ML to advance materials science. Building on this potential, significant progress is being made at the Advanced Light Source (ALS) to integrate ML tools into various synchrotron applications, including tomography segmentation, autonomous scattering analysis, and multimodal data fusion. Efforts are focused on implementing ML as a service, simplifying adoption by providing web-based solutions designed for seamless use across facilities. These tools aim to enable reliable and scalable ML applications for tasks such as the segmentation of complex 3D tomography datasets and automated experimental feedback in scattering experiments. This talk will explore the evolving role of ML at synchrotrons while addressing key challenges.

CPP 30.2 Wed 16:45 H34

Deep Learning-Driven GISAXS Data Processing for Nanostructure Characterization — •Yufeng Zhai[1], Shachar Dan[1], Julian Heger[2], Peter Müller-Buschbaum[2], and Stephan Roth[1,3] — [1]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Notkestr. 85, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, Garching 5, Germany — [3]Royal Institute of Technology (KTH), Stockholm, Sweden

Nanostructured materials, are at the forefront of advanced applications in various fields, owing to their unique physical and chemical properties. Grazing incidence small-angle X-ray scattering (GISAXS) has emerged as a powerful technique for probing the morphology of these nanostructures, offering valuable insights into electron density distributions both at the surface and within thin films. In our approach, we first simulate GISAXS pattern using the Distorted Wave Born Approximation (DWBA) model to generate high-quality training datasets. We then apply deep learning techniques, specifically convolutional neural networks (CNNs), to predict size distributions from GISAXS data. Our results demonstrate that CNNs are highly robust under varying noise conditions and present a promising, time-efficient approach for overcoming the challenges of conventional scattering analysis. This study highlights the potential of integrating advanced computational methods and new analytical tools to enhance the characterization of nanostructures.

CPP 30.3 Wed 17:00 H34

Towards Closing the Autonomous Loop at Multiple Facilities: Developing Web-based User Interfaces and Data Infrastructure for Autonomous Experiments and Automated Data Reduction Workflows — •Benedikt Sochor[1,2], Wiebke Koepp[2], Tanny Chavez[2], Runbo Jiang[2], Dylan McReynolds[2], Marcus Noack[3], Raja Vyshnavi Sriramoju[2], Aidan Coffey[2], Ronald Pandolfi[3], Eric Schaible[2], Chenhui Zhu[2], Frank Schlünzen[1], Stephan V. Roth[1,4], Alexander Hexemer[2], and Sarathlal Koyiloth Vayalil[1,5] — [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]Applied Mathematics and Computational Research Division, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, 94720, CA, USA — [4]KTH Royal Institute of Technology, Teknikringen 56, 100 44 Stockholm, Sweden — [5]UPES, Applied Science Cluster, 248007 Dehradun, India

This project focuses on establishing a robust infrastructure for autonomous scattering experiments at two different synchrotrons: X-ray scattering beamlines at PETRA III (DESY, Hamburg) and at the Advanced Light Source (ALS, Berkeley), initially beamline P03, the micro- and nano-focus small- and wide-angle X-ray scattering beamline (MiNaXS) at DESY, and the SAXS/WAXS/GISAXS/GIWAXS beamline 7.3.3 at the ALS. For selected science cases, the infrastructure's capabilities to handle large datasets during time-resolved and scanning X-ray scattering experiments will be highlighted.

CPP 30.4 Wed 17:15 H34

Imaging techniques for characterization of organic photonic devices utilizing digital luminescence — •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

The generally spin-forbidden T_1-S_0 transition of organic molecules gives access to pronounced long-lived room temperature phosphorescence in surprisingly many molecules, but is easily quenched by environmental oxygen. Controlling and utilizing these competing processes has led to the development of digital luminescence as a photonic design principle and its usage in programmable luminescent tags (PLTs) for application in sensing and information storage. To study and utilize this persistent luminescence, a spatially and temporal resolved imaging technique allows us to extend the characterization of these phenomena beyond spectroscopic measurements. By analyzing high-resolution images, differences in intensity and activation time within a single PLT can be detected, allowing conclusions as to structural irregularities. Evaluating each pixel individually also provides great insight into the statistical distribution of these values without the extensive need for samples and measurements. Thus, imaging techniques offer an excellent extension to the characterization of material systems for digital luminescence and by that allowing us to understand and optimize structure-property relationships. This represents an important step towards the use of PLTs for information storage and exchange.

CPP 30.5 Wed 17:30 H34

3D Nanoprinted Polarization Optics Directly on Optical Fibers — •Tim Stechel — Leibniz Institute of Photonic Technology, Albert-Einstein-Str. 9, 07745 Jena, Germany

Polarization is a fundamental property of electromagnetic radiation, influencing numerous areas of physical sciences and optical technologies. Developing functional interfaces that seamlessly integrate polarization control with fiber optics opens new opportunities for advancing these technologies. Using two-photon polymerization, we fabricate 3D structures on the sub-micron scale, directly on optical fibers. This high-resolution additive manufacturing technique enables the creation of tailored microstructures that can precisely control the polarization state of light as it enters and exits fibers. These custom interfaces are highly adaptable to different fiber types and optical configurations, allowing for enhanced polarization shaping and analysis. In this talk, we present the design process, fabrication process and characterization of the fabricated structures. Our approach combines the versatility of 3D printing with the precision required for nanoscale optical engineering, providing a robust platform for research into light-matter interactions and advancing fiber-based photonic technologies. Potential applications span diverse fields, from telecommunications to advanced optical metrology, demonstrating the broad impact of integrating 3D-printed microstructures with fiber optics.

CPP 30.6 Wed 17:45 H34

Phase-cycling and double-quantum two-dimensional electronic spectroscopy using a common-path birefringent interferometer — Daniel Timmer[1], •Daniel C. Lünemann[1], Moritz Gittinger[1], Antonietta De Sio[1], Cristian Manzoni[2], Giulio Cerullo[2], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität Oldenburg, Germany — [2]Politecnico di Milano, Italy

Ultrafast coherent spectroscopy techniques provide unique insights into the coherent dynamics of atomic, molecular and solid state quantum systems. For this, an experimentally challenging but all the more powerful technique is two-dimensional electronic spectroscopy (2DES), which allows to selectively probe coherent and incoherent couplings and to isolate individual excitation pathways by controlling the absolute phases of the ultrashort optical pulses that interact with the system (phase-cycling, PC). Its experimental implementation can be greatly simplified by employing birefringent in-line interferometers (TWINS) which are inherently phase stable. However, TWINS

is so far considered to be incapable of this phase control. Here, we demonstrate PC capabilities for 2DES using an adapted TWINS interferometer by recording rephasing, non-rephasing, zero-quantum and double-quantum 2DES on a molecular J-aggregate. This extension is easy to implement and enables new experimental capabilities for TWINS-based 2DES in multidimensional all-optical and photoemission spectroscopy and microscopy.
[1]: D Timmer, DC Lünemann, et al., Optica (accepted, DOI: 10.1364/OPTICA.543007)

CPP 30.7 Wed 18:00 H34

Real-time structure-transport investigation under mechanical strain in flexible carbon-based conductive polymer nanocomposites — •Sarathlal Koyiloth Vayalil[1,2], Vaishnav B[2], Benedikt Sochor[1], Stephan V. Roth[1,3], Ajay Gupta[2], Tobias Kraus[4,5], and Debmalya Roy[6] — [1]Deutsches Elektronen-Synchrotron DESY, 22607, Hamburg, Germany — [2]Department of Physics, Applied Science cluster, UPES, Dehradun 248007, India — [3]Division of Coating Technology, KTH Royal Institute of Technology, 100 44 Stockholm, Sweden — [4]INM Leibniz-Institute for New Materials, 66123 Saarbruecken, Germany — [5]Colloid and Interface Chemistry, Saarland University, 66123 Saarbruecken, Germany — [6]DMSRDE, Kanpur 208013, India

In this work, an in situ ultra-small angle X-ray scattering combined with electrical transport measurements under mechanical strain has been carried out in flexible, conductive carbon polymer nanocomposite to observe the real-time structural variations in nanofiller morphologies and distribution. For this purpose, the non-polar and polar elastomers viz. polydimethylsiloxane and polyurethane respectively, loaded with 0D Carbon black, 1D Carbon nanotubes, and 2D Graphene has been employed. The study has elucidated that, it is the filler′s fractal dimension that varies rather than aggregate distribution upon stress that decides PNC′s electrical conduction. Further, a novel relationship has been established between fractal dimension and composite′s conductivity, which invincibly guides in designing wearable and flexible conductors.

CPP 30.8 Wed 18:15 H34

In Situ Synchrotron X-Ray Computed Tomography Studies of Specialty Optical Fibers — •Ali Karatutlu[1], Zehra Gizem Mutlay[1], Andriy Budnyk[1], Gianluca Iori[2], Philipp Iori[3], and Bülend Ortaç[1] — [1]Bilkent University, Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM), Ankara, 06800 Turkey — [2]Paul Scherrer Institute PSI Forschungsstrasse 111 5232 Villigen PSI Switzerland — [3]SESAME - Synchrotron-light for Experimental Science and Applications in the Middle East, Allan, 19252, Jordan

Specialty fibers have complex structures due to their geometry, including glass core and cladding, multilayered polymer coatings, and the variations of their elemental compositions. Such complex structures of the specialty and microstructured fibers with air holes and the deformation due to manufacturing fiber lasers during fiber splicing can be investigated by X-ray computed tomography (XCT). The fiber fabrication process includes deposition and post-processes with a subsequent fiber drawing. Here, we present the first official results performed at the station BEATS, SESAME, for the synchrotron XCT imaging of specialty optical fibers all in one, such as polarization-maintaining, active, and photonic crystal fibers. In addition, temperature-dependent XCT measurements provided information on how inner structures, such as polymer coatings, could evolve for PM fibers. The conditions of the XCT measurements and the inner structure of the same type of fibers were found to be crucial and act as the guidelines that will be presented for the structures with sizes close to the voxel size.

CPP 31: Responsive and Adaptive Polymers

Time: Wednesday 16:15–18:00 Location: H38

Invited Talk CPP 31.1 Wed 16:15 H38

Moving with minimum effort – Optimal work protocols for systems with memory — •Sarah Loos[1], Samuel Monter[2], Felix Ginot[2], and Clemens Bechinger[2] — [1]DAMTP, University of Cambridge, UK — [2]University of Konstanz

Energy optimization is crucial in engineering and may also govern nonequilibrium processes in chemical and biological systems. Finding optimal solutions for microscale processes–dominated by thermal or nonthermal fluctuations and often displaying memory effects arising from internal degrees of freedom or coupling to viscoelastic environments–posses additional challenges, necessitating general guiding principles. We demonstrate such a general principle for the fundamental problem of dragging a harmonic trap containing a single particle over a finite distance within a given time while minimizing work input. We show that the optimal dragging protocol and the corresponding mean particle trajectory both exhibit time-reversal symmetry, which is a universal and exclusive feature of the optimal solutions. The symmetry principle holds across all media described by a linear generalized Langevin equation, irrespective of the memory kernel or noise properties, including glassy, granular, and active media. For intrinsically driven systems, such as active particles, we show that the optimal protocols remain identical to those for passive systems, but work fluctuations are always increased [2]. [1] S.A.M. Loos, S. Monter, F. Ginot, and C. Bechinger, Phys. Rev. X 14, 021032 (2024). [2] R. Garcia-Millan, J. Schüttler, M.E. Cates, and S.A.M. Loos, ArXiv:2407.18542 (2024).

CPP 31.2 Wed 16:45 H38

Influence of Azobenzene Moieties on the Swelling Behavior of Poly(Dimethylacrylamide) Films in Water Vapor under UV-Irradiation — •David P. Kosbahn[1], Julija Reitenbach[1], Morgan P. Le Dû[1], Lukas V. Spanier[1], René Steinbrecher[2,3], André Laschewsky[2,3], Robert Cubitt[4], and Peter Müller-Buschbaum[1] — [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

This study investigates the swelling behavior of p(AzAm-co-DMAm) films in both isomeric states of the photoswitchable molecule azobenzene (Az). The impact of UV irradiation on swelling in water vapor is examined, with the aim of controlling water uptake, expansion, and nanoscale morphology. This material shows potential for applications in light sensors, photo-actuators, and drug delivery systems. We employ time-resolved FTIR spectroscopy to monitor group vibrations during swelling and irradiation, gaining insights into molecular interactions throughout the isomerization process. Additionally, in situ time-of-flight neutron reflectometry on a thin film provides time- and depth-resolved data on the water distribution along the surface normal. The results shed light on the influence of azobenzene moieties on the polymer's microscopic properties.

CPP 31.3 Wed 17:00 H38

Critical analysis of adhesion work measurements from AFM-based techniques for soft contact — Dmitrii Sychev[1,2], Simon Schubotz[1,2], Quinn A. Besford[1], Andreas Fery[1,3], and •Günter K. Auernhammer[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]TU Dresden, Germany — [3]Chair of Physical Chemistry of Polymeric Materials,TU Dresden, Germany

The work of adhesion is a thermodynamic quantity that is frequently measured by atomic force microscopy (AFM). Its determination requires quasi-equilibrium measurements. Here, we address the question of to what extent atomic force microscopy qualifies for quasi-equilibrium measurements. To measure the work of adhesion, we combined soft colloidal probe AFM (SCP AFM) with reflection interference contrast microscopy (RICM). We extract the work of adhesion either from the pull-off force or from the contact radius to measure the adhesion behavior of poly(N-isopropylacrylamide) (PNIPAM) polymer brushes in the swollen and solvent-induced collapsed state. In the swollen state, the adhesion to the PNIPAM brush was fivefold larger and exhibited significant time dependencies when measured with SCP AFM. A strong rate dependence of the pull-off force method was indicative of a non-equilibrium process. In order to reliably determine the equilibrium work of adhesion, the contact radius method was found to be the better because it is not rate dependent. In summary, using optical measurements to determine the contact radius is beneficial when deriving the works of adhesion between colloidal probes and polymer brush surfaces.

CPP 31.4 Wed 17:15 H38

Chain conformation of thermo- and photo-responsive polymers — •Peiran Zhang[1], René Steinbrecher[2], Cy M. Jeffries[3], André Laschewsky[2], Peter Müller-Buschbaum[1], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Institute of Chemistry, University of Potsdam, Potsdam-Golm, Germany — [3]European Molecular Biology Laboratory, DESY, Hamburg, Germany

Endowing thermoresponsive polymers with additional photoresponsivity is of interest for applications such as drug delivery and soft robotics, owing to the non-invasive nature of these stimuli and the high temporal and local resolution of the photostimulus. The lower critical solution temperature (LCST) behavior in aqueous solution, characterized by a coil-to-globule transition at the cloud point (CP), can be finely tuned by incorporating photoswitches. Among these, azobenzene (AB) is the most widely used due to its pronounced trans-cis isomerization without side reactions. However, due to the weak change of dipole moment, its influence on the CP is only small. To enhance this photo effect, we used various amino acids as flexible linkers between the thermoresponsive backbone and the AB moiety. Dynamic light scattering reveals that a higher AB content leads to a larger shift of the CP, while small-angle X-ray scattering indicates that the amino acid linker reduces the influence of the inherent rigidity of the AB side groups, making the entire polymer chain more flexible. This approach allows adjusting the CP in wide ranges of temperature, thereby enhancing the range of applications.

CPP 31.5 Wed 17:30 H38

Acoustic levitation for dynamic studies of poly(N-isopropylacrylamide) microgels at the air-water interface — •Atieh Razavi[1], Regine von Klitzing[1], Romain Bordes[2], and Amin Rahimzadeh[1] — [1]Soft Matter at Interfaces, Institute for condensed Matter Physics, Technical University of Darmstadt, Hochschulstraße 8, 64289 Darmstadt, Germany — [2]Applied Surface Chemistry, Chalmers University of Technology, Gothenburg, Sweden

Acoustic levitation provides a unique platform for studying the surface dynamics of an air-water interface covered with poly(N-isopropylacrylamide) (PNIPAM) microgels. By utilizing standing acoustic waves, droplets are trapped at nodal positions, creating a contact-free environment to examine the effects of microgel stiffness, droplet evaporation, and amplitude modulation on droplet deformation. The research focuses on quantifying the aspect ratio (AR) of levitated droplets as a function of frequency of amplitude modulation, microgel concentration, and cross-linker content over time. In addition, we modulate the amplitude of the acoustic pressure at different frequencies (0.005 Hz0 to 05 Hz) to get insight into the interfacial rheology. With this new method, we can qualitatively characterize the interfacial behavior of microgels at the air-water interface such as the elastic modulus of the interface and adsorption kinetics[1].

CPP 31.6 Wed 17:45 H38

Structure and dynamics in injectable hydrogels from thermoresponsive triblock terpolymers — •Feifei Zheng[1], Pablo A. Álvarez Herrera[1], Wenqi Xu[1], Joachim Kohlbrecher[2], Sohila Abdelhafiz[3], Anna P. Constantinou[4], Theoni Georgiou[4], Aristide Dogariu[3], and Christine M. Papadakis[1] — [1]Technical University of Munich, TUM School of Natural Sciences, Garching, Germany — [2]Paul Scherrer Institut, Villigen, Switzerland — [3]CREOL, University of Central Florida, Orlando, USA — [4]Imperial College London, Department of Materials, London, UK

Block copolymers with blocks featuring lower critical solution temperature behaviour have attracted great interest for 3D bioprinting because they form a runny solution at room temperature, but a hydrogel at body temperature. The structure of the solution and the hydrogel as well as dynamic information and their changes upon gelation process are essential for understanding. Here we address an ABC triblock terpolymer consisting of a hydrophilic A block, a hydrophobic B, and a thermoresponsive C block. The results from small-angle neutron scattering on 15 wt% polymer solutions indicate that ABC form spherical core-shell micelles, that transform into cylinders in the gel state and form a more compact structure upon heating. By the combination of dynamic light scattering (DLS) and spatiotemporal coherence-gated DLS measurements, the dynamic information of gelation process was retrieved, which reveals the thermoresponsive C block contracts and the micelles aggregate to from the gel upon heating.

CPP 32: Poster Session II

Time: Thursday 9:30–12:00 Location: P3

CPP 32.1 Thu 9:30 P3

Influence of Salt Addition on the Ionic Conductivity, Hydration Behavior, and Structure of Poly(sulfobetaine) Hydrogels for Electrolyte Applications — •Friederike Ganster[1], Marcell Wolf[2], Gilles Wittmann[2], Peter Müller-Buschbaum[1], and Lucas P. Kreuzer[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), 85748 Garching, Germany

Polyzwitterionic hydrogels are promising candidates for electrolytes in aqueous solid-state batteries, such as zinc-ion batteries (ZIBs), due to their ability to retain water molecules that facilitate ionic transport. The retained water acts as a lubricant, coordinating with the charged groups of the polyzwitterion and reducing interactions with mobile Zn^{2+} ions, thereby promoting the dissociation of ions and improving ion mobility. We systematically investigate how the addition of cosmotropic $ZnSO_4$ or rather chaotropic Zn(acetate) affects the ionic conductivity of poly(sulfobetaine)-based hydrogels. Our findings reveal that while ionic conductivity is generally increased, the extent and nature of this enhancement strongly depend on the specific salt type. We attribute this to unique and salt-type sensitive structural and hydration changes. X-ray scattering techniques resolve the electrolyte structure, and FTIR and Raman spectroscopy provide insights into the altered hydration behavior. Electrochemical impedance spectroscopy correlates these structural and hydration changes with variations in ionic conductivity and ion transport efficiency.

CPP 32.2 Thu 9:30 P3

Exploring pressure effects on the coil-globule transition of a pH sensitive polymer — •Ved Mahajan, Varun Mandalaparthy, and Nico F. A. van der Vegt — Technical University, Darmstadt

Macromolecules like polymers and proteins are essential to everyday life, with their structure and function influenced by environmental changes. The coil-globule transition is ubiquitous and is influenced by factors like hydrophobic interactions. External conditions, such as pressure, impact this transition differently in proteins and thermoresponsive polymers like PNiPAM[1].

This study investigates the effect of pressure on the coil-globule transition of a pH-sensitive hydrophobic polymer using constant-pH molecular dynamics. Our Results show that both pH and pressure significantly influence the transition. While pressure and charge both cause chain swelling, charge counteracts pressure-induced chain extension at high pressure. We observe distinct water structuring around positively and negatively charged sites with consequence to the polymer's pressure response. Additionally, we explore zwitterionic polymers under pressure, providing insights into biologically relevant secondary structures.

[1] Papadakis, C. M.; Niebuur, B.-J.; Schulte, A. Thermoresponsive Polymers under Pressure with a Focus on Poly(N-isopropylacrylamide) (PNIPAM). Langmuir 2024, 40 (1), 1* 20, DOI: 10.1021/acs.langmuir.3c02398

CPP 32.3 Thu 9:30 P3

Microscopic Insights into NaTFSI Based Thermoelectric Polymer Electrolyte by Raman Spectroscopy — •Julian-Steven Schilling[1] and Jens Pflaum[1,2] — [1]University of Wuerzburg, 97074 Würzburg — [2]Center for Applied Energy Research (CAE Bayern e.V.), 97074 Würzburg

The variety of chemical components, solution-based processability, and intrinsically low thermal conductivity have positioned polymers as leading materials in the field of organic thermoelectrics. Since materials facilitating ionic transport provide significantly higher thermoelectric voltages compared to electronic ones, we have analyzed the thermoelectric transport properties of a methacrylate-based solid polymer electrolyte. This study pursued our previous work [1] on this solution processed electrolyte by revealing new insights into the interaction of the conducting NaTFSI salt and the polymer backbone on microscopic length scales. By means of Raman spectroscopy, we use e.g. the S-C stretching modes and their salt concentration dependency to identify free TSFI Ions inside the polymer matrix which are responsible for the thermoelectric properties. In addition, we highlight the concentration dependent characteristics of the liquid versus solid electrolyte phase as well as the impact of the photoinitiator used for UV-curing on the electrolyte behaviour. [1] arxiv:2403.09340

CPP 32.4 Thu 9:30 P3

Ion Transport in Block Copolymer Electrolytes: Insights from Atomistic MD Simulations — •Jignesh Dhumal[1], Diddo Diddens[2], and Andreas Heuer[3] — [1]IGS BACCARA, Universität Münster — [2]Helmholtz Institute Münster (IEK-12), Forschungszentrum Jülich GmbH — [3]Institut für physikalische Chemie, Universität Münster

Electrolytes are essential in batteries to facilitate ion transport between electrodes. Block copolymer electrolytes, have emerged as a promising class due to their high ionic conductivity and enhanced mechanical strength. However, despite several experimental and computational studies demonstrating their significance, an atomistic-level understanding of ion transport in Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI)-doped polystyrene-block-poly(ethylene oxide) (PS-b-PEO) block copolymers remain limited. In this study, we employ atomistic molecular dynamics simulations over extended timescales up to a microsecond examining the structural stability of the polymeric system and determine ion co-ordination within. We also quantify ion dynamics and transport properties in the PEO bulk region and the behavior at the PS/PEO interface, providing new insights into the mechanisms governing ion transport in this material.

CPP 32.5 Thu 9:30 P3

Advanced Synchrotron Characterization of NDI based acceptor thin films — •Subhalakshmi Suresh Kumar[1,2], Eva M. Herzig[1], and Christopher R. McNeill[2] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]McNeill Research Group, Department of Materials Science and Engineering, Monash University, Wellington Road, Clayton, Victoria, 3800 Australia

The transition to renewable energy has brought polymer solar cells (PSCs) to the forefront due to their lightweight, flexible, and environmentally friendly properties. The alignment of conjugated polymers within PSCs is critical for improving charge transport and overall device performance. This study aims to enhance the alignment of NDI-based acceptor thin films by employing fabrication methods such as blade coating and post-treatment annealing. Thin films were methodically prepared by varying coating speeds, substrate temperatures, and annealing conditions, followed by characterization using UV-Vis spectroscopy, Near-Edge X-ray Absorption Fine Structure (NEXAFS), and Grazing Incidence Wide-Angle X-ray Scattering (GIWAXS). The analyses demonstrated a significant enhancement in molecular alignment after annealing, particularly in PNDITBT films, which showed pronounced backbone alignment. These findings highlight the potential of synchrotron-based techniques in optimizing thin-film microstructures, paving the way for the production of highly efficient laminated organic solar cells with bilayer heterojunctions.

CPP 32.6 Thu 9:30 P3

Morphologies in Thin Films of Charged Pentablock Terpolymers During Solvent Vapor Annealing — •Yujia Gu[1], Constantinos Tsitsilianis[2], and Christine M. Papadakis[1] — [1]TU Munich, TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]University of Patras, Department of Chemical Engineering, Patras, Greece

Thin films from block copolymers containing charged blocks offer enhanced possibilities for precise structural modulation. In our previous work on thin films from a symmetric ABCBA pentablock terpolymer with cationic B and C midblocks and hydrophobic end blocks A, the pH-dependent degree of ionization of the charged midblocks was found to significantly influence the thin-film morphology [1]. In this study, we explore the possibilities to tune the thin film structures during solvent vapour annealing (SVA) using the same ABCBA pentablock terpolymer. Spin-coated films are prepared at various pH values and are subjected to SVA using selective solvents. Depending on the solvent selectivity, SVA may alter the film structure, e.g. by promoting reorganization toward equilibrium morphologies. We utilize in-situ atomic force microscopy (AFM) and spectral reflectometry (SR) to monitor structural transitions during SVA. By systematically examining the effects of pH and solvent selectivity, this study aims to provide insights into controlling nanostructure morphology in charged pentablock copolymers, with implications for advanced thin-film design.

CPP 32.7 Thu 9:30 P3

Adaptive Air-Water Interfaces with Spiropyrans and Arylazopyrazoles — •Michael Hardt[1], Javier Carrascosa-Tejedor[2], Philipp Gutfreund[2], Richard A. Campbell[3], and Björn Braunschweig[1] — [1]University of Münster (Germany) — [2]Institut Laue-Langevin (France) — [3]University of Manchester (UK)

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. Using molecular switches that respond to orthogonal triggers, the properties of fluid interfaces can be preconditioned, and a low level of adaptivity can be integrated, extending the possibilities of soft matter interfaces beyond responsive functions. We explore the adaptive behaviour of air-water interfaces decorated by spiropyran (SP) and arylazopyrazole (AAP) photo-responsive surfactants. When exposed to UV light, the SP surfactants become more surface active, while the AAP surfactants undergo E/Z photoisomerization, significantly reducing their surface activity. By adjusting the intensity and duration of the UV exposure, the interfacial properties can be shifted from a simple responsive state (upon weak UV irradiation) to a more complex conditioned response (upon intense UV irradiation), accompanied by a dramatic alteration in interfacial chemistry. Vibrational sum-frequency generation (SFG) and neutron reflectometry suggest that prolonged UV exposure induces SP and AAP surfactant aggregation at the air-water interface, driving the conditioned response where thick SP layers up to 5 nm form in the presence of Z-AAP.

CPP 32.8 Thu 9:30 P3

Is Anomalous Underscreening Detectable via AFM? — •Esther Ohnesorge, Thomas Tilger, Michalis Tsintsaris, 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 gain 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 anomalous 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 aqueous salt solutions. We systematically varied the type of salt, the surface chemistry of the confining surfaces (silica vs mica) as well as their curvature to bridge the gap between CP-AFM and SFA.

CPP 32.9 Thu 9:30 P3

Dynamic Wetting of Adaptive Polyelectrolyte Substrates: A multiscale approach — •Mona Meltschoch, Tünde Benedek, and Regine von Klitzing — Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

Wetting phenomena are of great importance across various scientific disciplines and the wettability dynamics of adaptive substrates, such as polyelectrolyte (PE) multilayers (PEM), have gained significant attention. An interesting property of PE substrates is their propensity to swell in a liquid environment. However, complexities like the disparity between time and length scales make experimental investigations quite challenging. We prepared PE substrates by the layer-by-layer method, with a focus on their wettability at the nanoscale. We used atomic force microscopy (AFM) as the main characterisation technique. An optical contact angle (CA) tensiometry method is used for macroscopic measurements, layer thickness is determined by ellipsometry and X-ray reflectometry (XRR). Previous results show a decrease in water CA on silicon wafers coated with polystyrene sulfonate (PSS) as outermost layer in water-saturated atmosphere. To investigate the dependence on thickness, chain length and charge of the outer layer, different PEMs were fabricated and characterised. Here, the substrates were investigated with an AFM and showed to exhibit smooth surfaces while linearly increasing in thickness. The decrease in water CA is more pronounced with an increasing thickness and differs if PSS or PAH are outermost layer.

CPP 32.10 Thu 9:30 P3

Molecular Imprinting of PEDOT in Polyelectrolyte Multilayers — •Martin Hunger, Muhammad Khurram, Sven Neuber, and Christiane A. Helm — martin.hunger@uni-greifswald.de

Electrically conductive films of Poly(3,4-ethylenedioxythiophene): poly(styrenesulfonic acid) (PEDOT:PSS) are formed by sequential adsorption of oppositely charged macromolecules. PEDOT:PSS serves as polyanion, and PDADMA is the polycation. When the top layer is PEDOT:PSS, the electrical conductivity is large (8 kS/m), when the top layer is PDADMA, the electrical conductivity is three orders of magnitude lower. In addition, vis-IR absorption spectroscopy shows that the PEDOT density in PEDOT:PSS-terminated films is high, while it is low in PDADMA-terminated films. When a PDADMA layer is adsorbed, turbidity measurements of the adsorption solution show that PEDOT diffuses out of the film. This can be explained entropically: a few PDADMA molecules with many positive charges replace many small molecules with few positive charges. Furthermore, exposure to solutions with divalent or trivalent cations reduce the conductivity of PEDOT-PSS-terminated films. We discuss whether PSS returns to previous binding sites upon adsorption of PEDOT:PSS, a behaviour that is typical for molecular imprinting.

CPP 32.11 Thu 9:30 P3

Extension of initiated chemical vapor deposition to new polymers via silylation — •Lynn Schwäke[1], Artjom Businski[2], Thomas Strunskus[1], Franz Faupel[1], Rainer Herges[2], and Stefan Schröder[1] — [1]Chair for Multicomponent Materials, Department of Materials Science, Kiel University, 24143 Kiel, Germany — [2]Otto Diels Institute of Organic Chemistry, Kiel University, 24143 Kiel, Germany

Initiated Chemical Vapor Deposition (iCVD) is a powerful technique for the solvent-free and conformal deposition of polymer thin films on sensitive substrates and complex geometries. The utilisation of a variety of monomers enables the fabrication of films with specifically tailored properties and functionalities. However, the evaporation of monomers is a prerequisite for iCVD processes. Consequently, this limits its applicability, for example, in the synthesis of hydrogels. The hydrophilic nature of potential monomers and the presence of other strong intermolecular interactions result in low vapor pressures, which in turn hinders their use in iCVD. A well-known strategy, e.g. in the context of drug detection by gas chromatography-mass spectrometry (GC-MS), is silylation, which is used to weaken inter-molecular forces. Here silylation was employed to enhance the vapor pressure of hydrophilic 2-hydroxyethyl methacrylate (HEMA), an important monomer in the synthesis of hydrogels. Consequently, silylation is proposed as a general route for the introduction of low vapor pressure monomers into iCVD systems, which would lead to a significant expansion of the available monomer toolbox.

CPP 32.12 Thu 9:30 P3

In-Situ Neutron and Raman spectroscopy on polymer thin films at varying humidity — •Marcell Wolf[1], Lucas Kreuzer[1], Friederike Ganster[2], Christopher Garvey[1], and Peter Müller-Buschbaum[2] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany — [2]Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Frank-Straße 1, 85748 Garching, Germany

Here we present a new sample environment for in-situ neutron and Raman spectroscopy on polymer thin films at varying humidities and temperatures. The combination of in-situ Raman and neutron spectroscopy shows the advantage that no difference within the sample composition, temperatures and humidity variations at the sample can be neglected, compared to separated single measurements. The structural changes can be directly related to the dynamic changes while varying the environment. We plan to describe our setup and present the first results of this new sample environment measured at the neutron time-of-flight spectrometer FOCUS at the PSI, Switzerland. For our knowledge this is the first time, that both spectroscopy techniques in comibination with varying humidity are applied at in-situ measurements. The new sample environment will be available to all users at time-of-flight spectrometer TOFTOF at the MLZ, as soon as the reactor restarts. Different variations of the sample cell, especially designed for different neutron experiments are available at other neutron instruments at the MLZ.

CPP 32.13 Thu 9:30 P3

Second order nonlinear optical properties of hexagonal boron nitride nanosheets h-BNNs — •Dina Atwa Khalil and G. Omar — Laser Institute for Research and Applications, Beni-Suef University, Egypt

The superior optical characteristics of hexagonal boron nitride nanosheets (h-BNNs) have been drawing more attention in the past few years. However, scientists have not yet thoroughly studied the nonlinear optical (NLO) properties of such innovative material. Here, NLO characteristics of h-BNNs are investigated for the first time utilizing the Z-scan approach that had been irradiated with 100 fs laser pulses using different excitation wavelengths that started from 740 to 820 nm at a constant incident power of 1 W. The studied 2D nanomaterial was prepared by a straightforward and effective technique for producing (h-BNNs), which is mechanical exfoliation. Their morphology and crystal structure have been investigated using different techniques, including UV-vis spectroscopy, scanning electron microscopy (SEM), transmission electron microscopy (TEM), and Raman spectroscopy. The measurements of nonlinearity show that by increasing the excitation wavelength, the nonlinear absorption coefficient decreases in a linear trend. The as prepared h-BNNs performed fascinating optical limiting with excellent two-photon absorption. This innovative optical nanomaterial makes them promise for sensitive optical components and laser protection applications.

CPP 32.14 Thu 9:30 P3

Highly oxidized Graphene Oxide as a Drug Delivery platform: Functional Group Interactions and Controlled Release Mechanisms — •Codrut Costinas[1], Liviu Cosmin Cotet[2], Monica Baia[1], Klara Magyari[3], and Lucian Baia[1] — [1]Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania — [2]Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, Cluj-Napoca, Romania — [3]Interdisciplinary Research Institute on Bio-Nano-Sciences, Babes-Bolyai University, Cluj-Napoca, Romania

Graphene oxide (GO) presents a promising platform for drug delivery, given its versatile surface chemistry and high surface area that enable effective drug loading and controlled release. Our study investigates the capabilities of an in-house produced, highly oxidized GO as a carrier by examining its interactions with two model compounds: methylene blue and methyl orange, as well as two drugs: doxorubicin and gentamicin sulfate. Through spectroscopic investigations (UV-VIS, FT-IR, and Raman), potentiometric titrations, and drug loading and release experiments we successfully identify the functional groups and bond types involved in drug-GO interactions in different pH media, most notably hydrogen bonding, electrostatic interactions, and π-π stacking. Furthermore, by taking into consideration the pKa values between GO acidic groups and the drugs ionizable groups, we can estimate both loading and pH-responsive release behavior in simulated physiological pH conditions. These findings highlight the flexibility of GO as a drug carrier, supporting its application in the development of customizable drug delivery systems for various therapeutic needs.

CPP 32.15 Thu 9:30 P3

Electronic Properties of a Naphthalene Diimide (NDI)-based Covalent Organic Framework (COF) — •Johann Olbrich[1], Laura Fuchs[1], Bibhuti Bhusan Rath[2], Bettina V. Lotsch[2], and Frank Ortmann[1] — [1]TUM School of Natural Sciences, Technische Universität München, Germany — [2]Nanochemistry Department, Max-Planck-Institute for Solid State Research, Stuttgart, Germany

Covalent organic frameworks (COFs) are a versatile class of porous polymers that exhibit exceptional tunability and electronic properties, making them attractive for various applications including water splitting [1], solar batteries [2] or other optoelectronic applications.

We investigated the electronic properties of a naphthalene diimide (NDI)-based COF, which demonstrates robust photoinduced charge separation in aqueous environments, by using density functional theory (DFT) calculations. We provide theoretical insights into the stability of the charges in NDI-based COFs under hydrated conditions, highlighting their potential for advanced electronic and material applications. For this, we determined the formation of a stable radical on the NDI unit through the addition of a hydrogen atom. Further modeling of interactions of small water clusters with the COF indicated the emergence of a radical anion on the NDI, accompanied by the stabilization of H+ in an H2O cluster.

[1] K. Gottschling, G. Savasci, H. Vignolo-González, S. Schmidt, C. Ochsenfeld, and B. V. Lotsch, J. Am. Chem. Soc. 2020, 142, 12146.

[2] Y. Wang, Y. T. Chan, T. Oshima, V. Duppel, B. V. Lotsch, J. Am. Chem. Soc. 2024, 146(37), 25467-25476.

CPP 32.16 Thu 9:30 P3

Lithium Distribution Heterogeneity in the Graphite Anode of 21700-Type Cylindrical Li-Ion Cells during Aging — Dominik Petz[1,2], •Peter Müller-Buschbaum[2], and Anatoliy Senyshyn[1] — [1]Heinz Maier-Leibnitz-Zentrum (MLZ), 85748 Garching, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Electrochemical cycling in lithium-ion batteries involves an active exchange of lithium ions and electrons between the cathode and anode materials. In addition to material properties, this exchange is influenced by cell parameters such as electrode dimensions and geometry, current density, temperature, pressure, reaction rate, and others. These parameters are generally neither uniformly distributed nor static, thereby contributing to the stabilization of heterogeneous states in Li-ion batteries, typically seen in the lithium concentration distribution across the electrodes.

Previous studies have shown that, with cell aging, the distribution of lithium ions in the graphite anode of 18650-type lithium-ion batteries shifts over time. In this study, the heterogeneity of a fresh and an aged 21700-type Li-ion battery was examined using multiple diffraction techniques with both synchrotron and neutron radiation. Laboratory-based techniques such as SEM and incremental capacity analysis were also employed. The findings revealed a notable lithium distribution after cell aging, prompting the question of how cell format impacts cell aging behavior.

CPP 32.17 Thu 9:30 P3

Steering sulfur reduction kinetics of lithium-sulfur batteries by interfacial microenvironment modulation — •Cheng Yuan[1,2], Liang Zhang[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou 215123, China

Catalytic conversion of lithium polysulfides (LiPSs) is considered as an effective avenue to suppress the shuttle effect of lithium-sulfur (Li-S) batteries, for which the interfacial microenvironment constructed by the interaction between electrocatalysts and LiPSs plays a pivotal role in modulating the sulfur reduction kinetics. However, most of previous reports mainly focused on modulating the band structure of electrocatalysts or LiPSs alone to enhance the catalytic activity rather than considering the interfacial microenvironment as a whole. Herein, we propose a binary descriptor composed of the energy difference between d-band of electrocatalysts and p-band of LiPSs ($\Delta\epsilon$M-S) and the antibonding filling degree (ϵABF), which capture the energy band contributions from both electrocatalysts and LiPSs, to reveal the influence of interfacial microenvironment on sulfur reduction kinetics. Among different designed electrocatalysts, NiO presents a moderate LiPSs anchoring capacity and rapid electron transfer kinetics owing to the optimal $\Delta\epsilon$M-S and decreased ϵABF after interacting with LiPSs, which lead to a robust interfacial microenvironment and thus guarantee a continuous catalytic conversion of LiPSs in the long-term cycling.

CPP 32.18 Thu 9:30 P3

Polymer of intrinsic microporosity as the silicon-based anode electrode additive — •Ming Yang[1], Ruoxuan Qi[1], Ya-Jun Cheng[2], Yonggao Xia[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Ningbo Institute of Materials Technology & Engineering, Chinese Academy of Sciences, 1219 Zhongguan West Rd, Ningbo, 315201, Zhejiang Province, P. R. China

Silicon-based anodes are promising alternatives due to their high theoretical specific capacity and low voltage platform to traditional graphite anodes for high-energy-density lithium-ion batteries (LIBs). However, their performance is significantly hindered by silicon's substantial volume expansion during cycling, which often leads to electrode degradation. Therefore, it is crucial to design a robust electrode structure and establish a stable solid electrolyte interface (SEI) to address these challenges. Herein, an intrinsic microporosity polymer PIM-COOH is prepared, which has good compatibility with the polyacrylic acid (PAA) binder as a silicon-based anode additive. The microporous structure of the PIM-COOH molecule can effectively improve the transport of lithium ions and improve the electrochemical kinetics. In addition, due to the inherent microporous properties of PIM-COOH additives, the affinity between the electrode and the electrolyte is enhanced. As a result, good lithium-ion transport and mechanical integrity are maintained, resulting in improved long-term stability and high-rate performance.

CPP 32.19 Thu 9:30 P3

In-situ interface film forming on the high-voltage LiCoO2 cathode by a tiny amount of nanoporous polymer additives — •Ruoxuan Qi[1], Ming Yang[1], Tianle Zheng[1], Xingchen Liu[2], Yonggao Xia[2], Ya-Jun Cheng[2,3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]NIMTE, CAS, Zhejiang Province, P. R. China — [3]College of Renewable Energy, Hohai University, Jiangsu Province, P. R. China

The LiCoO2 (LCO) cathode has been foreseen 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 from 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 modulates 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 the cyclic stability and improving the rate performance, providing new perspectives for the electrodes fabrication and improving LCO-based high-energy-density cathodes.

CPP 32.20 Thu 9:30 P3

Ionic transport race between lithium and sodium in non-aqueous electrolytes — •Chinwendu Nancy Anabaraonye[1,2], Diddo Diddens[3], and Andreas Heuer[1,3] — [1]Institute of Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster, Germany — [2]International Graduate School for Battery Chemistry, Characterization, Analysis, Recycling and Application (BACCARA), University of Münster, Corrensstr. 40, 48149 Münster, Germany — [3]Helmholtz Institute Mnster (IEK-12),Forschungszentrum Jülich GmbH, 48149 Münster,Germany;

The need to meet the storage requirements of energy systems safely and efficiently has led to research into electrolytes other than the commonly used lithium-ion batteries. While the lithium-ion battery is the clear market leader, there is increasing interest in sodium-ion batteries, which are cheaper and more abundant. The present work is a comparative study of the transport properties of lithium hexafluorophosphate ($LiPF_6$) and sodium hexafluorophosphate ($NaPF_6$) in carbonate electrolytes consisting of ethylene carbonate (EC) and ethyl methyl carbonate (EMC). Using molecular dynamics simulations, we analyse the influence of EC ratio and salt concentrations on the solvation structure and how this affects the ionic transport properties such as diffusivity and ionic conductivity of the system. Our results show higher conductivity and diffusivity of Na compared to Li for the analysed systems. Optimal ionic conductivity for Na was achieved above 1 M concentration, in contrast to Li. Overall, we observed differences in the coordination and mobilities of lithium and sodium cations.

CPP 32.21 Thu 9:30 P3

3D Electrodeposition of Porous Cu for long-cycling Lithium-Metal Batteries — •Lyuyang Cheng[1], Zhuijun Xu[1], Tianle Zheng[1], Yingying Yan[1], Fabian Apfelbeck[1], Yuxin Liang[1], Ya-jun Cheng[2], and Peter Müller-buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Hohai University, 213022 Changzhou, China

Lithium (Li) metal is the ultimate anode for rechargeable batteries. Its high specific capacity (3860) 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 nano WAXS images with lithium growth, which can help to explain the mechanism. We also provide a feasible method to fabricate the porous Cu cathodes with different electrodeposition solution concentrations.

CPP 32.22 Thu 9:30 P3

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

All-solid-state lithium-ion batteries (ASSLIBs) are the most promising power sources for high-safety and high-energy-density energy storage devices. However, the practical application of ASSLBs has been hindered by poor interfacial stability and inferior ionic conductivity. Herein, a layered-double-hydroxide (LDH) reinforced poly(ethylene oxide) (PEO) composite polymer electrolyte is designed, which delivers a wide electrochemical window, high ionic conductivity, and superior Li+ transference number with a low LDH loading. The Li symmetric cells show ultra-long cycling stability at 0.1 mAh/cm2. The all-solid-state Li//LiFePO4 exhibits an excellent cycling stability with a high capacity retention of 90.1% at 0.1 C over 250 cycles. Furthermore, the structure-activity relationship between the component structure of the electrolyte and the electrochemical performance was elucidated by operando nanofocus wide-angle X-ray scattering (nWAXS).

CPP 32.23 Thu 9:30 P3

Organic polyaniline-based cathode materials — •Meriem N. Boudjenane[1], Friederike Ganster[2], Sebastian Mühlbauer[1], and Lucas P. Kreuzer[1] — [1]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), 85748 Garching, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Organic cathode materials feature tuneable structures, abundant active sites, and compatibility with multivalent charge carriers, thereby allowing to overcome challenges typically faced in inorganic cathode systems such as structural instability, and environmental hazards. We focus on the development of polyaniline (PANI) based cathodes. PANI, a conductive polymer, has demonstrated high capacity, excellent rate capability and fast ionic diffusion. Cellulose-based materials such as carboxymethyl cellulose (CMC) are used as binders and enhance the overall stability and electrochemical performance. By tuning parameters such as material composition, ionic strength, water content, and temperature, we elucidate how the conductivity and electrochemical stability of the PANI-based cathode can be optimized. Advanced techniques like X-ray diffraction, scanning and transmission electron microscopy, and electrochemical analysis provide deep insights into the structure-function relationship of the cathode materials while operando Raman spectroscopy will give insights into the charge/discharge mechanism and respective redox reactions, guiding the development of high-performance organic cathodes.

CPP 32.24 Thu 9:30 P3

Consistent Electrostatics in Bottom-Up Modeling of Electrode-Fluid Systems: Determining the Capacity from Ab-Initio to Continuum Models — •Philipp Stärk[1,2], Henrik Stooss[3], Philip Loche[4], and Alexander Schlaich[3] — [1]Stuttgart Center for Simulation Science (SC SimTech), University of Stuttgart, 70569 Stuttgart, Germany — [2]Institute for Computational Physics, University of Stuttgart, 70569 — [3]Institute for Atomistic Modeling of Materials in Aqueous Media, Hamburg University of Technology, 1073 Hamburg, Germany — [4]Laboratory of Computational Science and Modeling, IMX, Ecole Polytechnique Federale de Lausanne,1015 Lausanne, Switzerland

Detailed understanding of electro-catalysis, batteries and supercapacitors, often requires modeling these systems on an atomistic scale. However, at this length scale and level of detail, most continuum assumptions about electrodes are clearly no longer valid. This is problematic for physical models and methods of analysis which rely on concepts from continuum electrostatics. We demonstrate in this work that a realistic Constant Potential Method model based on DFT data for gold can still consistently be described by concepts of continuum electrostatics, provided the electrostatic boundary condition is modeled correctly. Furthermore, we apply this description to determine the dielectric behavior of water in nanoporous gold. We systematically investigate the difference between conducting and inert confinement on the static dielectric response.

CPP 32.25 Thu 9:30 P3

Evaluating the Impact of Electrode Defects on PEMFC Performance and Durability — •Faezeh Mehdizadeh siahroudi[1], Sebastian Prass[1], and Andreas Bett[2] — [1]Division Hydrogen Technologies Department Fuel Cell Fraunhofer Institute for Solar Energy Systems ISE 79110 Freiburg, Germany — [2]Fraunhofer-Institut für Solare Energiesysteme ISE

According to previous research, imperfect membrane electrode assembly (MEA) manufacturing processes can lead to catalyst layer and membrane defects. Therefore, we have decided to investigate the impact of missing areas in cathode and anode electrodes on the performance and durability of polymer electrolyte fuel cell (PEMFC). Missing areas with varied sizes and configurations are used to determine a threshold at which a missing area can be considered as a crucial defect that degrades MEA components. In our work, several in-situ electrochemical techniques were used, including polarization curves, linear sweep voltammetry (LSV), cyclic voltammetry (CV), and electrochemical impedance spectroscopy (EIS) experiments. The structural changes in the electrodes and the membrane are visualized through SEM cross-sectional imaging.

CPP 32.26 Thu 9:30 P3

Hybrid electrolyte LLZO/PEO-systems: Impact of salt concentration and temperature on the structural properties close to the interface — •Laura Hölzer[1], Melania Kozdra[2], Daniel Brandell[2], and Andreas Heuer[1] — [1]Institut für physikalische Chemie, Universität Münster, Corrensstr. 28-30, 48149 Münster, Germany — [2]Department of Chemistry - Ångström Laboratory, Uppsala University, Box 538, 75121 Uppsala, Sweden

Composite electrolytes are an opportunity for creating new and improved materials as ideally they combine the advantages of different types of electrolytes. One example for this being the LLZO/PEO-system. Insights into the properties and dynamics at and around the interface can be gained by looking at the system with atomistic simulations. Previously it could be seen that over the course of a simulation there is a movement of the Li^+ ions into the crystal.[1] Here, we analyse under which conditions equilibration is possible on the simulation time scales. Molecular dynamic simulations are performed. Three different concentrations and temperatures between 400K and 700K are studied. One could see the formation of a well-defined structure around the interface, which includes an additional layer of Li ions on both sides of the crystal that in equilibrium at 700K is independent of concentration, indicating structure formation via strong enthalpic driving forces. Furthermore, interesting insight into the reorganization of the polymer and the salt due to the presence of the LLZO can be gained.

[1] Kozdra, M.; Brandell, D.; Araujo, C. M. G.; Mace, A. Physical Chemistry Chemical Physics 2024, 26, 6216-6227.

CPP 32.27 Thu 9:30 P3

Structural investigation of lithium deficient metal chlorides solid electrolytes — •Francesco Falsina — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

The strong demand for new and emerging sustainable energy solutions to address climate change and the requirements for increased high energy and power density have positioned solid-state batteries as a key research area. Lithium metal chlorides (LiMCl) are considered as promising candidates for next-generation batteries due to their high ionic conductivity, thermodynamic stability, and favourable mechanical properties. In this study, we investigated Li(3-3x) M(1+x)Cl6 compounds with M = Dy, Ho, Tb, and Tm using X-ray diffraction (XRD), confirming that all samples crystallize in the space group P3m1, though exhibiting partial crystallinity and high disorder without post-synthesis annealing. The effect of lithium deficiency was explored on the ionic conductivity employing Electrochemical Impedance Spectroscopy (EIS), offering further insights into their potential for solid-state battery applications.

CPP 32.28 Thu 9:30 P3

Morphology and intracrystalline dynamics of semicrystalline polyester Poly(3-hydroxy-2,2-dimethylbutyrate)

— •Johann C. Holz[1], Arman Edalat[1], Kay Saalwächter[1], Thomas Thurn-Albrecht[1], and Eugene Chen[2] — [1]Martin-Luther-University, Halle, GER — [2]Colorado State University, Fort Collins, USA

Semicrystalline polymers are classified as crystal-fixed (non-diffusive) or crystal-mobile (diffusive) based on polymer chain mobility within the crystal. Crystal-fixed polymers exhibit lower crystallinity, thinner lamellae ($d_a > d_c$), and less variation in thickness ($\sigma_a > \sigma_c$). Finding a biodegradable alternative for crystal-mobile polyethylene (PE) remains a priority for sustainable research. Poly(3-hydroxybutyrate) (P3HB), a biodegradable polyester, was recently found to be crystal-mobile, but suffers from poor mechanical properties.

We here study Poly(3-hydroxy-2,2-dimethylbutyrate) ($P3H(Me)_2B$), a structurally similar polyester with methyl-groups substituted for the two α-hydrogens, to improve mechanical toughness, thermal stability, and recyclability. Our analysis of $P3H(Me)_2B$ by Small-Angle X-ray Scattering (SAXS) revealed that it crystallizes in a crystal-fixed mode. This finding contrasts with the crystal-mobile behavior observed in P3HB. Wide-Angle X-ray Scattering (WAXS) corroborated the crystal structure that has already been described in literature, while also revealing previously undetected diffraction peaks. Furthermore, Nuclear Magnetic Resonance (NMR) spectroscopy enabled precise quantification of the polymer's crystallinity, facilitating accurate determination of the melting enthalpy H_f for a 100% crystalline sample.

CPP 32.29 Thu 9:30 P3

Optical properties of biosynthesized nanoscaled Eu_2O_3 for red luminescence and potential antidiabetic applications

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This contribution reports on the optical properties of biosynthesised Eu_2O_3 nanoparticles bioengineered for the first time by a green and cost effective method using aqueous fruit extracts of Hyphaene thebaica as an effective chelating and capping agent. The morphological, structural, and optical properties of the samples annealed at 500°C were confirmed by using a high-resolution transmission electron microscope (HR-TEM), x-ray diffrac tion analysis (XRD), UV-Vis spectrocopy, and photoluminescence spectrometer. The XRD results confirmed the characteristic body-centered cubic (bcc) structure of Eu_2O_3 nanoparticles with an average size of 20 nm. HRTEM revealed square type morphology with an average size of ≈6 nm. Electron dispersion energy dispersive x-ray spectroscopy spectrum confirmed the elemental single phase nature of pure Eu_2O_3. Furthuremore, the Fourier transformed infrared spectroscopy revealed the intrinsic characteristic peaks of Eu-O bond stretching vibrations. UV-Vis reflectance proved that Eu_2O_3 absorbs in a wide range of the solar spectrum from the VUV-UV region with a bandgap of 5.1 eV. The luminescence properties of such cubic structures were characterized by an intense red emission centered at 614 nm. It was observed that the biosynthesized Eu_2O_3 nanoparticles exhibit an efficient red-luminescence and hence a potential material as red phosphor.

CPP 32.30 Thu 9:30 P3

Green synthesis of nanocellulose for archaeological wood preservation: a case study of cheops' second solar boat

— •Ihab Abdelbaki — Cairo University, Egypt

The preservation of ancient wooden artifacts presents significant challenges due to environmental degradation and biological deterioration. This study addresses these challenges through the development of an eco-friendly nanocellulose-based preservation method, specifically targeting the deterioration observed in the second solar boat of king khufu (cheops), one of egypt's most significant archaeological wooden artifacts. Nanocellulose was synthesized via a green approach using controlled acid hydrolysis of agricultural waste cellulose, followed by mechanical ultrasonication. the degradation assessment of the second solar boat revealed severe biological infestation, structural weakening, and dimensional instability, particularly in areas exposed to fluctuating humidity levels. The prepared nanocellulose, characterized by TEM, FTIR and XRD, exhibited crystallite sizes of 20-30 nm and a crystallinity index of 82%. when applied to degraded wood samples from similar archaeological contexts, the nanocellulose treatment demonstrated significant improvements in mechanical strength (40% increase), dimensional stability (65% reduction in swelling), and biological resistance. Importantly, the treatment maintained the artifact's aesthetic and historical integrity while providing a sustainable, reversible preservation solution. this study presents a promising green approach for the conservation of ancient wooden artifacts, offering implications for cultural heritage preservation worldwide.

CPP 32.31 Thu 9:30 P3

Investigation of photoelectrochemically induced degradation of III-V nanowires

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Over the past two decades, nanoscale structures like III-V nanowires (NWs) have become versatile components in electronic and photonic applications [1]. The large surface-to-volume ratio of NWs enhances reaction efficiency by providing more active sites for light-driven processes. To explore NWs' potential in photoelectrochemical solar energy conversion, we investigated their optoelectronic behavior. First, GaAs NWs were grown via Vapor-Liquid-Solid growth mode using Metal-Organic Vapor Phase Epitaxy. We performed Linear Sweep Voltammetry measurements where the III-V sample was brought into direct contact with the electrolyte. However, a major challenge is the degradation in performance due to the limited durability of NWs in electrolytes compared to planar surfaces. To evaluate the corrosion of NWs in electrolytes, we analyzed the NW structures before and after two hours of stability testing measurements by Scanning Electron Microscopy. Our results indicate that under continuous illumination no significant degradation besides surface roughening is observed while samples under chopped illumination, are nearly completely etched, with few or no NWs remaining intact.

[1] J. Koch et al., Adv. Mater. Interfaces 9, 2200948, 2022.

CPP 32.32 Thu 9:30 P3

Fabrication of Gas Sensors with High Sensitivity to NO_2 Based on Photoactivation of Porous Carbon Materials

— •Laura Pascual[1], Berta Pérez-Román[2], Jesús López-Sánchez[2], M. Alejandra Mazo[2], Álvaro Peña[3], David G. Calatayud[4], Daniel Matatagui[3], and Fernando Rubio-Marcos[2] — [1]Instituto de Catálisis y Petroleoquímica (ICP-CSIC), Madrid, España — [2]Instituto de Cerámica y Vidrio (ICV-CSIC), Madrid, España — [3]Instituto de Magnetismo Aplicado, (IMA-UCM-ADIF), Madrid, España — [4]Departamento de Química Inorgánica, Universidad Autónoma de Madrid (UAM), Madrid, España

The rise in gas emissions harms public health, with nitrogen dioxide (NO_2) being particularly dangerous due to its impact on the lungs and respiratory conditions. This emphasizes the need for highly selective gas sensors capable of detecting concentrations below 1 ppm in real time, while being miniaturised and operable at room temperature (RT).

Carbon-derived materials from carbides (CDC) are created through high-temperature chlorination, achieving surface areas over 2000 m^2/g. These materials feature hierarchical porosity (micro- to mesopores) and abundant active sites that support redox reactions for NO_2 detection. Incorporating heteroatoms improves charge transfer and electron-hole trap formation. The results show exceptional selectivity and sensitivity to NO_2, with detection below 1 ppm and room temperature operation using UV excitation (275 nm).

CPP 32.33 Thu 9:30 P3

Bimetallic Core-Shell-Nanoparticles for enhanced Raman spectroscopy

— •Moritz Willems[1], Steffi Stumpf[1,2], and Stephanie Hoeppener[1,2] — [1]Jena Center for Soft Matter (JCSM) — [2]Institute of Organic and Macromolecular Chemistry (IOMC)

Bimetallic Core-Shell-Nanoparticles have emerged as a versatile tool for advanced sensing applications, particularly in surface-enhanced Raman spectroscopy and tip-enhanced Raman spectroscopy. The combination of two metals in a Core-Shell configuration enhances the plasmonic properties and allows for extended plasmonic bandwidths, as well as superior electromagnetic field amplification in comparison to the monometallic nanoparticles. Silver nanoparticles have been demonstrated to offer effective enhancements for Raman spectroscopy. However, they do present certain challenges, including a narrow spectral range, poor chemical stability, and a relatively short lifespan. The coating of silver nanoparticles with a thin gold shell promises precise control over localised surface plasmon resonance, expanding spectral ranges for Raman spectroscopy measurements, especially between the peaks of gold and silver, by changing the relative thickness of the shell. Furthermore, the gold coating allows for measurements in water, while also providing a prolonged lifespan. The synthesis of these nanoparticles utilizes chemical reduction by microwave irradiation, providing fast, energy efficient and uniform heating. Various methods have been tested to overcome the problems of synthesising a gold shell on silver, and detailed transmission electron microscopy and UV-Vis spectroscopy analysis complement the Raman spectroscopy results.

CPP 32.34 Thu 9:30 P3

Classical simulation studies of dissociation equilibria in nanoconfined systems — •Kira Fischer, Henrik Stooss, and Alexander Schlaich — Institute for Atomistic Modeling of Materials in Aqueous Media, Hamburg University of Technology, Germany

Dissociation equilibria in nanoconfinement are relevant to the chemistry of nanostructured catalysts, aerosols and protein pockets. Experiments indicate that nanoconfinement affects the dissociation of water, however to date a comprehensive understanding is still lacking. Here, we investigate dissociation equilibria in nanoconfinement from a classically. Using molecular dynamics and free energy methods we study hydrochloric acid in diamond nanoconfinement in the dilute limit at ambient conditions.

Our studies reveal a depletion of hydrochloric acid in nanoconfinement, with a negative excess by up to a factor of 100. The negative excess is attributed to the balance between hydronium adsorption and chloride depletion at the interface. Additionally, we propose that hydronium is adsorbed to the diamond interface by dipole orientation within a local electric field. Notably, in the smallest pore, the $\mathrm{p}K_\mathrm{a}$ is increased by 1. We also introduce useful concepts for analysing dissociation equilibria in confinement. This includes the chemical potential in confinement, which enables quantification of ionic excess in the dilute limit. Furthermore, we demonstrate how to derive the chemical potential from the potential of mean force, thereby decomposing the different energetic contributions to the excess chemical potential.

CPP 32.35 Thu 9:30 P3

Gas quenching under ambient conditions for efficient and stable inverted perovskite solar cells with surface treatment — •Zhaonan Jin, Xiongzhuo Jiang, Zerui Li, Xiaojing Ci, Guangjiu Pan, Kun Sun, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Inverted perovskite solar cells have gained significant attention due to their potential for high efficiency and stability. In the process, the active layer fabrication plays a key role in determining the performance of the solar cells. Gas quenching is an important technique in the preparation of perovskite solar cells as it enhances the film quality and solar cell performance by precisely controlling the crystal growth and minimizing defects. As for the post-treatment of the active layer, surface passivation plays a crucial role in enhancing the performance of perovskite solar cells by reducing surface defects of perovskite interfaces. This study explores the influence of different passivation materials on the morphology of perovskite films and the performance of gas-quenching assisted FA0.8Cs0.2Pb(I0.6Br0.4)3 solar cells. This work provides a practical solution for the production of low-cost and high-performance inverted perovskite solar cells while maintaining operational stability in real-world environments.

CPP 32.36 Thu 9:30 P3

Facet-dependent photovoltaic efficiency and stability variations in mixed Sn-Pb perovskite solar cells — •Xiaojing Ci, Xiongzhuo Jiang, Guangjiu Pan, Jinsheng Zhang, Zerui Li, Kun Sun, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Since the first breakthrough of perovskite solar cells using a solid-state structure, the solar cell power conversion efficiency has increased from 9.7% to 26%. These exciting improvements are mainly attributed to achieving a pinhole-free thin film at the beginning and an increased understanding of microstructures on perovskite thin films. In addition, the rapid PCE improvement has been accompanied by an increased understanding of microstructures on perovskite thin films. The photovoltaic performance of PSCs has been found to correlate strongly with their facet orientations. For example, the charge carrier lifetime, open-circuit voltage deficit and device hysteresis of PSCs are related to the structure and density in (111) crystal facets of perovskite. Besides, different crystal facets have different atomic arrangements and coordination, which lead to different atomic potential landscapes and, subsequently, to different electronic, physical, and chemical properties. Nevertheless, the deep understanding of perovskite thin films, especially the crystal facets of the thin film, still lags behind that of single-crystal samples or other inorganic thin films. In this work, we prepare the mixed tin-lead perovskite film with different orientations according to the facet engineering. We research the role of the different perovskite crystal facets in stability and optoelectronic properties.

CPP 32.37 Thu 9:30 P3

Processing-property relationships in printed hybrid halide perovskites — •Manuel Lippert[1], Meike Kuhn[1], Maximilian Spies[2], Anna Köhler[2], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]Optoelektronik weicher Materie, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

Solution processable hybrid halide perovskites solar cells have been extensively studied over the last ten years and great advances in efficiency have been achieved. An important factor for the performance of the final solar cell is the morphology of the perovskite layer. Therefore, control of structure formation mechanisms is highly desirable. [1] We investigate systematically the processing of the active layer to determine processing parameters that are decisive for structure formation. To reliably study the effect of time relevant processing steps on the perovskite layer, we use automated processing. Applying photoluminescence, optical microscopy and grazing incidence wide angle X-ray scattering (GIWAXS) allows us to determine the morphology on the nano and micron scale and detect the correlations between processing and efficiency.

[1] Meike Kuhn, Felix A. Wenzel, Christopher Greve, Klaus Kreger, Matthias Schwartzkopf, Hans-Werner Schmidt, Helen Grüninger, Eva M. Herzig, Tailored Supramolecular Additives to Control the Crystallization Process and Morphology of MAPbI3, *submitted*

CPP 32.38 Thu 9:30 P3

Simulating light induced phase separation in $\mathbf{MAPbBr_{1.8}I_{1.2}}$ perovskites — •Sebastian Schwartzkopff, Ivan Zaluzhnyy, Ekaterina Kneschaurek, Paul Zimmermann, Dmitry Lapkin, Hans Mauser, Alexander Hinderhofer, and Frank Schreiber — University of Tübingen

By changing the ratio of halides within mixed organic halide perovskites, such as $\mathrm{MAPbBr_{1.8}I_{1.2}}$ (MA -methylammonium), one can adjust the band gap. This is quite desirable for solar cell applications where precisely tunable bandgaps enable the creation of high efficiency solar cells. However, when illuminated with visible light, these materials undergo a phase separation into Br-rich and I-rich phases, which destroys the tuned band gap. To better understand; and hopefully control this process, we utilize phenomenological approaches, such as Cahn-Hilliard and Monte Carlo models, to simulate the light-induced phase separation. We compared the results of our simulations with the experimental diffraction data. Cahn-Hilliard simulations presented quite a few difficulties in replicating the observations. The Monte Carlo simulations on the other hand allow us to investigate the influence of various material parameters on the phase separation, such as iodine-to-bromine ratio, charge carrier density and intensity of illumination. In general, we found that Monte Carlo simulations with the right choice of model parameters are quite capable of reproducing the experimental observations.

CPP 32.39 Thu 9:30 P3

Enhanced Stability of Perovskite Solar Cells via Double-End Coupling Silane — •Xinwei Tian, Xiongzhuo Jiang, and Peter Müller-Buschbaum — TUM School of Natural Science, Chair for Functional Materials, 85748 Garching, Germany

Containing reactive triethoxysilyl groups, 1,4-bis(triethoxysilyl)benzol (BTEB) has high thermal stability by forming robust siloxane networks through hydrolysis and condensation reaction. Besides, BTEB has good hydrophobicity, so it can function as a protective barrier to prevent moisture ingression into the sample, which ensures long-term operation of the perovskite solar cells (PSCs). BTEB can also passivate the interface defect, thus reducing non-radiative recombination. On the other hand, because of the surface passivation effect of BTEB, a smoother and more uniform film layer can be obtained, which can enhance light absorption and reduce scattering loss effectively. In this way, the power conversion efficiency (PCE) can also be improved. In our work, we aim to apply BTEB as the interface modification material, ethyl acetate as antisolvent, to construct inverted perovskite solar cells with higher efficiency and stability.

CPP 32.40 Thu 9:30 P3

Morphology Control and Optical Modelling of $CsPbBr_3$ Nanocrystal Films for Emission Orientation Studies — •Lea Kolb, Roshini Jayabalan, and Wolfgang Brütting — Universität Augsburg, 86135 Augsburg, Germany

The remarkable properties of $CsPbBr_3$ perovskite nanocrystals, exhibiting a high photoluminescence quantum yield (PLQY) and a narrow emission linewidth with size- and composition-tunable bandgap, render them promising for the application as emitters in light-emitting diodes (LEDs). While PLQY and charge carrier transport for perovskite LEDs have been in the focus of extensive studies, the orientation of the emissive transition dipole moment (TDM) has not been investigated thoroughly yet. However, for TDM analysis, determining the complex refractive index of the nanocrystal films is crucial. In this work, variable angle spectroscopic ellipsometry (VASE) was used to obtain the optical constants of various samples containing $CsPbBr_3$ nanocrystals. To avoid scattering effects, VASE measurements require homogeneous films with minimal roughness. For this reason, the substrates on which the nanocrystal films were spin-coated had to be modified and the sample fabrication process was optimized. In order to describe the measured data accurately with optical fit models, the morphology and thickness of the films were studied comprehensively by atomic force microscopy (AFM). Finally, angular dependent photoluminescence (ADPL) measurements have been performed and modelled in order to obtain information about the TDM-orientation.

CPP 32.41 Thu 9:30 P3

PIN-type perovskite solar cells for space applications — •Ruodong Yang, Simon A. Wegener, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Perovskite solar cells have advantages such as low costs and high power-to-weight ratio, which render them to be promising candidates for space applications, where the mass is crucial for launch costs. In this study PIN-type solar cells are investigated. With its inverted p- and n-type structure, it has great research potential. However, solar cells in space also face challenges, such as vacuum, extreme temperature fluctuations during each orbit, and high radiation levels. The purpose of this study is to optimize the manufacturing procedure of PIN-type perovskite solar cells to address these challenges. We investigate the power conversion efficiency of the solar cells under similar environmental conditions to the low Earth orbit with illumination from an AM0 light source and thermal cycling by using optical microscopy to observe the structural changes during the operation. With the results of the measurements, the manufacturing procedure will be optimized, to determine the key factors to improve the performance and efficiency of PIN-type cells under space conditions.

CPP 32.42 Thu 9:30 P3

Perovskite solar cells temperature dependence under space-like conditions — •Anthony Vizcaino, Simon Alexander Wegener, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair of Functional Materials, 85748 Garching, Germany

In recent years, perovskites have attracted the scientific community's attention due to their properties and possible applications, making their use in solar cells one of the most relevant. Their high-power conversion efficiency, power-to-weight ratio, and manufacturing compared to the to-date used multi-junction devices make them a promising device for space applications, where it is possible to take advantage of all the intensity of sunlight that at the Earth*s surface is lost by absorption or scattering by the atmosphere. However, in this scenario, radiation and high temperatures would affect the solar cell. This study focuses on one of these problems and tries to understand how extreme temperatures and thermocycling through large periods of heating and cooling encountered in low Earth*s orbit affect perovskite solar cell performance and degradation. Operando studies allow to simulate thermal cycling conditions and measure the transmittance of solar cells, which combined with electrical characteristics from I-V measurements and active layer morphology from GIWAXS give us a robust knowledge of the temperature dependence of perovskite-based solar cells.

CPP 32.43 Thu 9:30 P3

In-situ Monitoring for Optimizing Perovskite Solar Cell Fabrication: Correlating Process Parameters with Power Conversion Efficiency — •Yuxin Liu, Alexander Tarasov, Maxim Simmonds, and Eva Unger — Department Solution Processing of Hybrid Materials and Devices, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany

Halide perovskite solar cells need dependable, reproducible production to reach commercialization. For stable perovskite photovoltaic manufacture and research, deposition processes must be monitored. In-situ photoluminescence (PL) monitoring compares the PL during spin-coating and annealing with absolute PL measurements obtained after annealing of the sample. Examples demonstrating how process conditions and variables like anti-solvent type and drip timing significantly influence PL signatures. We demonstrate that insight during processing can serve as feedback to stabilize the perovskite solar cell fabrication. In-situ PL monitoring shows two distinct peaks within one second of anti-solvent treatment, revealing perovskite nucleation and growth mechanism. All Helmholtz association perovskite PV research uses a standard operating procedure (SOP) for solar cell samples. Absolute PL measurements for thin-film samples quantify Quasi-Fermi Level Splitting, reflecting the opto-electronic quality of the absorber and losses at selective contacts. The absolute PL is correlated to the in-situ PL to establish how far in-situ PL during processing can predict solar cell performance. This study highlights the potential of optical process monitoring to enhance material and interface quality.

CPP 32.44 Thu 9:30 P3

The Construction of Temperature Gradient during Annealing to Guide Crystallization Direction — •Yiran Shi — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Perovskite solar cells have gained significant attention as promising candidates for next-generation photovoltaics due to their outstanding advantages. The quality of the perovskite layer is a crucial determinant of the efficiency and stability of photovoltaic devices. As a polycrystalline thin film, the size and compactness of crystals are key quality metrics, closely linked to the annealing process. Conventional annealing typically involves placing the thin film, post-nucleation, on a fixed-temperature heating platform for crystal growth. Without external guidance, crystallization usually progresses top-down, preferentially completing at the upper surface. This sequence often traps solvents within the film, hindering evaporation and leading to void formation, which negatively affects film quality and device performance. To address this issue, we propose an improved annealing strategy by introducing a vertical thermal gradient to guide a bottom-up crystallization process. This approach aims to delay top-surface crystallization, allowing solvents to escape more effectively and reducing void formation. From the results about SEM and GIWAX, it is improved film quality, with enhanced structural integrity and reduced defects, offering a pathway to optimize perovskite photovoltaic performance.

CPP 32.45 Thu 9:30 P3

Optimizing RbCsFAMA perovskite solar cells with piperazine-inspired passivation technique — •Bashudev Bhandari[1,2,3], Zekarias Teklu Gebremichael[1,2], Niklas Manikowsky[2,3], Chikezie Williams Ugokwe[1,2], Ulrich S Schubert[1,2], and Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-University Jena — [2]Faculty of Physics and Astronomy, Friedrich-Schiller- University Jena, Jena, Germany — [3]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller- University Jena, Jena, Germany

Perovskite solar cells (PSCs) have emerged as a promising photovoltaic technology, with extraordinary optoelectronic properties. However, stability and defects are the challenges of perovskite solar cells. This work explores the role of piperazine as a novel passivating agent to address these limitations. Piperazine's bifunctional structure enables effective defect passivation at the grain boundaries and interfaces of RbCsFAMA perovskite films, significantly reducing non-radiative recombination losses. Different characterization and imaging techniques photoluminescence spectroscopy, X-ray diffraction and scanning electron microscopy demonstrate improved crystallinity and electronic properties of the RbCsFAMA perovskite films after passivation. This improvement is shown to be transferred into solar cell devices.

CPP 33: Modeling and Simulation of Soft Matter IV

Time: Thursday 11:45–13:00 Location: H34

CPP 33.1 Thu 11:45 H34

Understanding COF/Electrode interfaces for electrocatalysis using DFT and molecular simulations — •Henrik Stooss[1], Philip Stärk[1,2], and Alexander Schlaich[1] — [1]Institute for Atomistic Modeling of Materials in Aqueous Media, Hamburg University of Technology, Hamburg — [2]SC SimTech, University of Stuttgart, Stuttgart

This study explores the complex dynamics at electrode/electrolyte interfaces under constant potential, crucial for advancing electrocatalysis and designing efficient energy systems, by combining advanced computational techniques to gain insights into mechanisms at these interfaces. We perform Density Functional Theory (DFT) simulations while maintaining a constant electrode potential. Despite challenges and computational costs, the DFT simulations provide insights into the electronic structure and behavior of electrode surfaces. We then parameterize a classical model based on the DFT data, enabling simulations of larger systems over longer timescales for comprehensive comparison with experimental ATR-SEIRAS data. This approach offers a detailed understanding of adsorption and transport phenomena at the electrode interface, potentially leading to better electrolyte compositions and improved electrode designs. This work advances the connection between first-principles calculations and experimental observations for material design.

CPP 33.2 Thu 12:00 H34

Porous microstructure of fibrous sheets in two transport regimes — Alexandra Serebrennikova[1], Phillip Gräfensteiner[2], Matthias Neumann[1], Volker Schmidt[2], Andoni Rodriguez[3], Peter Leitl[3], Werner Napetschnig[1], Ekaterina Baikova[1], Maximilian Fuchs[1], and •Karin Zojer[1] — [1]Graz University of Technology, Graz, Austria — [2]Ulm University, Ulm, Germany — [3]bionic surface technologies, Graz, Austria

In many applications, a porous material serves multiple functions. For example, paper sheets in packaging bags should allow excess air to escape quickly while minimizing moisture migration. Although the underlying physics are different, both transport processes depend on porosity. However, each function it is likely to be supported by additional, possibly different, microstructural properties. Can these microstructural properties be optimized for all functions or is this not possible due to inherently dependent properties? To answer this question for Stokes flow and reactive diffusive transport through paper, we simulate flow through μ-CT-determined microstructures using physics-informed neural networks, computational fluid dynamics, and pore network modeling. We combine these simulations with statistical morphological analysis including dependency quantification to provide the relevance and dependence of structural properties in both transport processes. Our study suggests that the two transport scenarios do not rely on the same set of structural properties, even when fiber swelling due to moisture transport is considered.

CPP 33.3 Thu 12:15 H34

Nuclear Quantum Effects in Clays — Sam Shepherd, Pawan Kurapothula, Nataly Realpe, Gareth Tribello, and •David Wilkins — Queen's University Belfast, Belfast, United Kingdom

Clay materials consist of layers, whose structure is heavily influenced by hydrogen-bonding interactions. Given the importance of nuclear quantum effects such as zero-point energy in water, a hydrogen-bonded liquid, a natural question to ask is how important these effects are in clays themselves.

I describe some work done by my group to understand the importance of nuclear quantum effects in clays and clay-water systems, and to interpret these effects in the same terms used to understand water. I also demonstrate a fully quantum-mechanical description of the interactions and dynamics in kaolinite clay.

CPP 33.4 Thu 12:30 H34

Protonated water clusters by stochastic approaches: probing machine learning resilience against quantum Monte Carlo noise — •Matteo Peria, Antonino Marco Saitta, and Michele Casula — Sorbonne Université, 4 place Jussieu Paris, France

A complete understanding of the hydrogen bond and proton transfer mechanism in water is still lacking, since it requires an accurate potential energy surface (PES) and very expensive quantum mechanical simulations of the nuclear part. Reproducing this high-dimensional surface with current high-level computational chemistry methods is infeasible for the largest clusters. We test gradient-based kernel ridge regression methods and neural networks to reproduce the PES starting from a dataset of energies and forces of the protonated water clusters obtained via simulations combining classical molecular dynamics (MD) for the nuclei and quantum Monte Carlo (QMC) for the electrons. The QMC+MD approach yields very accurate results for the classical dynamics, which are however affected by the intrinsic noise inherent in the stochastic sampling of both nuclear and electronic phase space. We prove that QMC multivariate noise is not necessarily detrimental to the learning of energies and forces and we determine under which conditions one can derive accurate and reliable MLIPs from QMC data.

CPP 33.5 Thu 12:45 H34

Effect of solid fillers on the thermodynamics and electrical properties of diblock copolymers and polymer blends. — •Alexander Chervanyov — University of Münster, Münster, Germany.

By making use of the developed theory we study the effect of solid fillers on the thermodynamics, phase behaviour and electrical properties of diblock copolymers (DBC) and polymer blends (PB). The theory relies on the combination of the liquid state approach, phase-field model for polymers, Monte-Carlo simulations, and the resistor random network model for fillers. Using the developed approach, we prove that the correlations imposed by the variations of the composition of PB cause a significant non-osmotic contribution to the polymer mediated interaction between fillers immersed in this blend. The effect of fillers on the stability and miscibility of compressible PB is studied in detail. We show that the presence of non-adsorbing fillers can be used to enhance the stability of a PB that shows low critical solution temperature (LCST) behavior. Finally, as an important practical application of the developed theory, we study the electrical response of an insulating DBC filled with conduictive fillers. In particular, the order-disorder transition in the host DBC system is found to be accompanied by the conductor-insulator transition in the filler network. The order-order transition between the lamella and cylindrical microphases of DBC proves to co-occur with a spike of the composite conductivity caused by restructuring of the conductive filler network.

CPP 34: Focus Session: Interactions Between Water and Cellulose I

Time: Thursday 15:00–16:00 Location: H34

Invited Talk CPP 34.1 Thu 15:00 H34

Understanding Nanocellulose-Water Interactions to Engineer Advanced Functional Materials — •Valentina Guccini — Uppsala University, Lägerhyddsvägen 1, Uppsala, Sweden

Water interactions are a central topic in the field of nanocellulose due to their pivotal role in nanocellulose's chemical reactivity, processability and physical properties. Yet, a key challenge that remains is bridging the fundamental understanding of nanocellulose-water interactions with the design and engineering of advanced functional materials. This presentation will address this challenge by summarizing the main characteristics of water-nanocellulose interactions and how these can be leveraged to engineer nanocellulose-based materials, in which water has both a structural and functional role. We will analyze the structure-property relationship in nanocellulose-based hydrogels, films and membranes for biotechnological and fossil-free energy applications (e.g. fuel cells and lithium-ion batteries). This presentation offers a new perspective on using nanocellulose-water interactions as a tool to enhance and tailor material performance and functionalities.

CPP 34.2 Thu 15:30 H34

Using Nanocellulose Hygroscopicity for Conductive 3D Paper Structures — •Marie Betker[1,2], Tim Erichlandwehr[3], Benedikt Sochor[1,4], Elisabeth Erbes[1,5], Yamit Alon[2], Alisher Kurmanbay[2], Yanan Li[6], Irene Fernandez-Cuesta[3], Peter Müller-Buschbaum[6], Simone Techert[1,5], Daniel Söderberg[2,7], and Stephan Roth[1,2,7] — [1]Deutsches Elektronen Synchrotron, Notkestrasse 85, 22607 Hamburg, Germany — [2]KTH Royal Institute of Technology, Teknikringen 56, 10044 Stockholm, Sweden — [3]Hamburg Advanced Research Centre for Bioorganic Chemistry, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [4]Lawrence Berkeley National Laboratory, 6 Cyclotron Rd, Berkeley, CA 94720, USA — [5]Institute for X-ray Physics, Goettingen University, Friedrich Hund Platz 1, 37077 Göttingen, Germany — [6]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [7]Wallenberg Wood Science Center, Teknikringen 52, 10044 Stockholm, Sweden

We report the fabrication of the, to this date, thinnest sprayed nanopaper foils. For that, we spray aqueous nanocellulose dispersions layer-by-layer on a hot substrate. The foils are only 2 um thin with an average basic weight of 1.9 g/square metre. We specifically exploit the hygroscopicity of paper-based materials to rearrange our water-soaked foils into three-dimensional, free-standing shapes. We further demonstrate the applicability of our foils by making them conductive via integration of silver nanowires. This approach is a step towards more sustainable, 3D organic electronics.

CPP 34.3 Thu 15:45 H34

A simulation study of the structure and mechanical properties of cellulose and callose hydrogels — •Robinson Cortes-Huerto[1], Nancy C. Forero-Martinez[2], and Pietro Ballone[1] — [1]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, DE — [2]Institut für Physik, Johannes Gutenberg-Universität, Staudinger 9, 55128 Mainz, DE

The cell wall of plants is a complex, self-organized and continuously evolving structure playing important roles in the life cycle of individual cells and the plant as a whole. It consists primarily of cellulose, which is the main responsible for its mechanical properties. Under environmental stress, a crucial role is played by callose, a polysaccharide closely related to cellulose and a minority component of the cell wall. A recent study (*Plant Signal. Behav.* **2019**, *14*, e1548878) suggested that the enhancement of mechanical properties by callose is due to its ability to order neighbouring water molecules, giving origin to solid-like water-callose domains. This hypothesis is tested by atomistic MD simulations using models representing cellulose and callose hydrogels. The results highlight systematic differences in the coordination and H-bonding of callose and cellulose by water, reflected in different dynamical properties of water in callose or cellulose hydrogels, partly validating the hypothesis. However, mechanical properties, characterized by the Young's modulus of the polysaccharide / water gels, are the same in callose/ and cellulose/water samples, suggesting that callose's ability to link cellulose nanofibres into networks is the main responsible for the strengthening of the plant cell wall.

CPP 35: Microswimmers and Microfluidics (joint session DY/BP/CPP)

Time: Thursday 15:00–17:45 Location: H37

Invited Talk CPP 35.1 Thu 15:00 H37

Light-Driven Manipulation of Passive and Active Microparticles — •Svetlana Santer — Institute of Physics and Astronomy, University of Potsdam, Germany

Chemical gradient near a solid/liquid can result in lateral long-range fluid transport termed diffusioosmotic (DO) flow. For instance, when photosensitive surfactant is irradiated with light converting the majority of the molecules in one of the possible isomers, emerging concentration gradient of isomers generates an osmotic pressure gradient tangent to the wall actuating the surrounding liquid to flow. [1-3] In my talk I will show how one can manipulate microparticles and even induce their self-propulsion by light urtilizing light driven diffusioosmotic (LDDO) phenomenon. Depending on the applied wave length one can either disperse/remove or gather particles. We will discuss how to establish light-driven hydrodynamics as a useful and versatile tool for investigating collective motion of self-propelled particles and aggregation

[1] Feldmann, D.; Maduar S.R.; Santer, M.; Lomadze, N.; Vinogradova O.I.; Santer, S. Scientific Reports, 6 (2016) 36443. [2] Santer, S. J. Phys. D: Applied Physics, 51 (2017) 013002. [3] Arya, P.; Umlandt, M.; Jelken, J.; Feldmann, D.; Lomadze, N.; Asmolov , E. S.; Vinogradova, O. I.; Santer, S. A. The European Physical Journal E, 44(50) (2021), 1-10.

CPP 35.2 Thu 15:30 H37

Regulated polarization of active particles in local osmotic flow fields — •Lisa Rohde, Desmond Quinn, Diptabrata Paul, and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, University Leipzig, Leipzig, Germany

Regulation in living systems is a fundamental principle for achieving robust functionality and maintaining specific non-equilibrium states. The control of certain properties and functionalities of systems on the microscale presents particular challenge since thermal fluctuations and environmental perturbations dominate. While synthetic active matter has demonstrated remarkable self-organization capabilities, examples of autonomous regulation processes at the single-particle level remain scarce. Here, we show experimentally that the interplay of two non-equilibrium processes leads to a regulated polarization state of active particles in local osmotic flow fields. Based on thermophoretic repulsive and attractive forces that are generated by a single heat source at the boundary, the active particles encircle the heat source at a stable distance depending on the heat source temperature. The balance of these temperature-induced processes causes a polarization of the active particles that is independent of the heat source temperature. The individual control of heat source and active particles in the experiment allows detailed investigation of the self-regulated polarization effect in which we find hydrodynamic interactions to dominate. As the effects rely on osmotic flows and phoretic interactions, we expect that the observed phenomena can be generalized to other active systems and flow fields.

CPP 35.3 Thu 15:45 H37

Active particle steering in three dimensions — •Gordei Anchutkin and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Leipzig University, Leipzig, Germany

Synthetic active particles serve as a model system that mimic the self-propulsion of living matter to explore fundamental aspects of non-equilibrium physics. Various collective phenomena of active agents have been studied, but mostly in the presence of hydrodynamic and physicochemical boundary effects. While theoretical works predict different collective dynamics in 3D, experimental investigations remain limited due the lack of experimental control over active swimmers in three dimensions.

Here we introduce three-dimensional control to the study of synthetic active matter. We demonstrate simultaneous control of thermophoretic microswimmers in 3D using single-particle tracking through digital holography and darkfield pattern tracking, with real-time wavefront shaping for steering. With the help of these experiments, we explore the interplay of thermophoretic propulsion, gravity, and optical forces for the active particles. By creating a three-dimensional active ensemble, we reveal how bulk interactions and boundary effects shape the collective behavior of active particles.

CPP 35.4 Thu 16:00 H37

***Trypanosoma brucei* in microchannels: the role of constrictions** — •Zihan Tan, Julian I. U. Peters, and Holger Stark — Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Trypanosoma brucei (*T. brucei*), a single-celled parasite and natural microswimmer, is responsible for the fatal sleeping sickness in infected mammals, including humans. Understanding how *T. brucei* interacts with fluid environments and navigates through confinements is crucial for elucidating its movement through blood vessels and tissues, and across the blood-brain barrier.

Using a hybrid multiparticle collision dynamics (MPCD)–molecular dynamics (MD) approach, we investigate the locomotion of an in-silico *T. brucei* in three types of fluid environments: bulk fluid, straight cylindrical microchannels, and microchannels with constrictions. We observe that the helical swimming trajectory of the in-silico *T. brucei* becomes rectified in straight cylindrical channels compared to bulk fluid. The swimming speed for different channel widths is governed by the diameter of the helical trajectory. The speed first slightly increases as the channel narrows and then decreases when the helix diameter is compressed. An optimal swimming speed is achieved when the channel width is approximately twice the bulk helix diameter. Furthermore, *T. brucei* notably slows down when entering the narrow constriction in a microchannel and strongly speeds up upon exiting due to a release of deformation energy of the straightened cell body.

CPP 35.5 Thu 16:15 H37

Helical motion of microorganisms can be more persistent than straight motion — •Leon Lettermann[1], Falko Ziebert[1], Mirko Singer[2], Freddy Frischknecht[2], and Ulrich S. Schwarz[1] — [1]BioQuant & Institute for Theoretical Physics, Heidelberg University — [2]Center for Integrative Infectious Disease Research, Heidelberg University

The movement of microorganisms has been extensively modeled by stochastic active particle models. In three dimensions, both swimming microorganisms, like sperm cells and some bacteria, and gliding microorganisms, like malaria sporozoites in the skin, often exhibit helical trajectories. If the internal driving force is the primary source of noise in the system, it induces random, yet time-correlated variations in the torque. To investigate this effect, we introduce a three-dimensional active rotational Ornstein-Uhlenbeck particle model. We find that the presence of a rotational component and the resulting helical path can mitigate the effect of intrinsic noise in the drive, allowing for larger long-time mean square displacements than straight movement at the same speed. The model not only provides qualitative insights into the constraints faced by microbes that may have led to the evolutionary selection of certain motility patterns, but also presents an analytical, quantitative tool for extracting information from these movements. We present and analyze corresponding data for malaria parasites gliding through hydrogels.

15 min. break

CPP 35.6 Thu 16:45 H37

Corrugated channels can filter ciliated microorganisms based on the metachronal wavelength — •Gonçalo Antunes and Holger Stark — Technische Universität Berlin, Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Many microorganisms (e.g. Paramecium) move by a carpet of cyclically beating cilia that cover their surface. These cilia often beat in an organized fashion, such that the beating phases form a traveling wave, referred to as a metachronal wave. In this study, we investigate the swimming of such microorganisms in corrugated microchannels. We model the motion of the cilia via a time-varying effective slip velocity applied on the microorganism's surface, which we approximate as an infinite slab. By employing the lubrication approximation, we show analytically that the swimming speed of ciliated microorganisms placed inside a corrugated channel is sensitive to the corrugation height, provided that the wavelength of the corrugation matches that of the metachronal wave. Indeed, the direction of motion itself may invert with respect to swimming in bulk fluid, with the channel acting as a virtual barrier which blocks microorganisms under specific conditions for corrugation and slip-velocity modulations, but allow others to pass through. We also show that the interplay between the corrugation and the slip velocity profile allows for the swimming of microorganisms with zero time-averaged slip velocity, which thus cannot swim in bulk fluid. Finally, we complement our theory with preliminary results from hydrodynamic simulations for radially-symmetric microorganisms of finite length in radially-symmetric corrugated channels.

CPP 35.7 Thu 17:00 H37

Motion of a single particle partially exposed in a simple shear flow — •Dominik Geyer[1,2], Aouane Othmane[1], and Jens Harting[1,2] — [1]Helmholtz-Institut Erlangen-Nürnberg for Renewable Energy (IET-2), FZ Jülich — [2]Department of Physcis, FAU Erlangen-Nürnberg

Sand immersed in the water can be imagined as a wet granular matter. Besides sedimentation, friction, and surface roughness are two relevant physical phenomes within this system. Many body systems in a turbulent regime have been studied using discrete elements methods for a long time, but a single particle in the Stokes flow regime is particularly interesting for biological systems and microfluidic devices.

A layer of quadratic-arranged spheres models the rough surface. The question arises of how to describe the motion of a single traveling particle over this substrate.

We choose a combined numerical and analytical approach. The Stokes equation is solved analytically for the sphere near a rough wall. Lattice Boltzmann simulations with momentum-exchange particle coupling are performed for different wall roughness and friction coefficients.

Although, the Stokes equation assumes that the particle Reynolds number is zero. Surprisingly, the numerical results match our theoretical description until a particle Reynolds number of two. In this regime, friction between the moving particle and the substrate significantly influences the angular velocity but has a minor influence on the traveling velocity in the flow direction.

CPP 35.8 Thu 17:15 H37

Rational Design of Smart Microfluidics in Responsive Channels — •Arwin Marbini — Albert-Ludwigs Universität Freiburg

Responsive microfluidics offers exciting potential for self-regulating biomimetic systems. This study explores bifurcating microchannel networks with pressure-sensitive resistances, combining experiments with simulations based on the Hagen-Poiseuille equation and a linear model. These methods extract critical, experimentally inaccessible parameters under steady-state and dynamic conditions. Our findings enable the design of adaptable microfluidic networks, unlocking precise flow control for future applications in biology, soft robotics, and advanced material systems.

CPP 35.9 Thu 17:30 H37

Blue Water: A passive, reusable microfiltration device for water purification — •Tim R. Baumann, Ioannis Gkekas, Martina Viefhues, and Dario Anselmetti — Experimental Biophysics, Bielefeld University

Water is the most vital resource for life on Earth. Due to pollution of freshwater and oceans, this valuable resource has become globally endangered. The effects of microplastic pollution are widely discussed in scientific, political, and socioeconomic contexts. Despite regulations on single-use plastics and microplastic output, efforts should also focus on reintegrating microplastics to achieve a sustainable circular economy. Furthermore, microplastic-sized particles can migrate through organic tissue and can therefore be classified as contaminants of emerging concern. However, filtering plastics of this size is a challenging task.

Thus, this work examines and extends the findings of Divi et al. regarding the suspension feeding mechanisms of various ray species. We studied the filtration performance and efficiency for different geometric ratios of channel widths in simulations and laboratory environments. First, we have the main inner channel connected to the pressure inlet. From this, two rows of tilted lamellae structures branch off laterally to the outer secondary channels.

By applying sufficiently high pressure ($> 6 \cdot 10^5\ Pa$) to the inlet and achieving flow and particle velocities of $> 35\ \frac{m}{s}$, we can purify 82 % of half of the initial fluid. To prevent rupturing of our microfluidic chip under this pressure, we further investigated using glass fiber reinforced PDMS and lowering the operating pressure.

CPP 36: Organic Electronics and Photovoltaics IV

Time: Thursday 15:00–16:00 Location: H38

CPP 36.1 Thu 15:00 H38

How to Capture and Release Fullerene from an Azobenzene-Bithiophene Nanolayer? — Dmitry A. Ryndyk and •Olga Guskova — IPF Dresden, Hohe Str. 6 01069 Dresden

Optimizing organic photovoltaic devices involves the strategic use of well-defined monolayers of azobenzene-bithiophene (Azo-BT) switches. These monolayers serve as a bridge between inorganic and organic components, allowing precise nanoscale control over electrode morphology [1]. Previous studies have demonstrated that cis- and trans-Azo-BT switches chemisorbed on a gold surface exhibit distinct geometrical, electronic, and charge transport properties. We further investigate the behavior of cis- and trans-Azo-BT monolayers, with a particular focus on ”nanotraps” nanometer-sized nanopores formed within the monolayers and their ability to capture&release fullerene. Our findings confirm that the photoswitchable ”closed” and ”open” configurations of Azo-BT nanotraps remain stable at room temperature under experimentally relevant surface densities. Energy calculations reveal that C60 molecules preferentially stabilize inside the open nanotrap near the pore surface, effectively capturing the fullerene. Additionally, a local energy minimum for C60 near the electron-donating BT block suggests charge transfer from the BT fragment to the fullerene, enhancing the interaction between the trap and the captured molecule. To expel the fullerene from the monolayer, we applied an alternating voltage electric field and determined the optimal parameters required to displace the nanoparticle, demonstrating the feasibility of controlled capture and release. [1] Savchenko, V. et al., Processes, 11 (2023) 2625.

CPP 36.2 Thu 15:15 H38

Deciphering vibronic interactions in NDI-T2 based donor-acceptor type oligomers with theoretical and experimental spectroscopy — •Maximilian F.X. Dorfner[1], Marko Medugorac[1], Ajeet Kumar[2], Jürgen Hauer[1], and Frank Ortmann[1] — [1]TUM School of Natural Sciences, Technische Universität München, 85748 Garching b. München, Germany — [2]Department of Chemistry, Lund University, Naturvetarvägen 14 222 62 Lund, Sweden

In this study, we investigate the alternating Naphthalendiimide-bithiophene co-oligomer (T2-NDI2OD-T2), a fundamental building block of the high charge-mobility polymer-semiconductor PNDI(2OD)2T. This class of materials has garnered significant attention for its exceptional charge transport properties, making it a promising candidate for applications in field-effect transistors and as non-fullerene acceptors in organic photovoltaics. We use Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT) to examine the ground and singlet excited state properties to understand the electronic structure and vibrational excitations. Additionally, we analyze the coupling between electronic and vibrational degrees of freedom by means of a Linear Exciton-Vibrational Coupling Model parameterized by DFT. We compare the computed optical observables to the experiment and discuss the role of molecular vibrations in this system.

CPP 36.3 Thu 15:30 H38

Grain Boundaries and Charge Mobility in Organic Semiconductors: A Non-Adiabatic Molecular Dynamics Approach — •Sonali Garg[1], Farhad Ghalami[1], Sebastian Schellhammer[2], and Marcus Elstner[1] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Technische Universität Dresden, Germany

Organic semiconductors have emerged as crucial materials in the development of electronic and optoelectronic devices due to their exceptional mechanical flexibility, lightweight nature, and cost-effectiveness. However, the presence of grain boundaries (GBs) can significantly impede device performance by introducing traps or potential barriers that reduce charge carrier mobility. This study investigates the influence of the GB characteristics, including misorientation angles and GB width, on charge carrier mobility and compares the results with intrinsic mobility. Non-Adiabatic Molecular Dynamics (NAMD) simulations, employing Fewest Switches Surface Hopping (FSSH) approach[1,2,3], were used to model charge transport dynamics. The charge transfer Hamiltonian was constructed using a fragment orbital approach, with its elements computed via the Density Functional Tight Binding (DFTB) method[4,5]. These insights provide a deeper understanding of the effects of GB on charge carrier mobility in organic semiconductors.

[1]Spencer. J et al. J. Chem. Phys. (2016) [2]Roosta. S J. Chem. Theory Comput. (2022) [3]Xie. W et al. J. Chem Theory Comput. (2020) [4]Elstner. M et al. Phys. Rev. B (1998) [5]Kubař. T et al. J. Phys. Chem. B (2010)

CPP 36.4 Thu 15:45 H38

Single-particle spectra of pentacene from exact simulations of Green’s functions in the time-domain — •Michel Panhans[1], Frank Ortmann[1], and Hiroyuki Yoshida[2] — [1]TUM School of Natural Sciences, Technische Universität München, 85748 Garching b. München, Germany — [2]Graduate School of Engineering, Chiba University, 1-33 Yayoicho, Inage-ku, Chiba, 263-0043, Japan

The investigation of single-particle spectra using experimental techniques such as photo-electron spectroscopy and inverse-photoelectron spectroscopy reveal the nature of the charge carriers close to the Fermi energy. In particular for organic crystals such as pentacene, the single-particle spectra are strongly affected by the electron-phonon coupling (EPC) and crucially deviate from the theoretical spectra based on ab initio band-structure calculations associated with the HOMO and the LUMO of the pristine crystal.

To model these experiments more accurately, Green’s-function approaches including the EPC are a suitable methodology to describe what is seen in experiments. In our present study, we calculated the HOMO and the LUMO spectra of pentacene single-crystals and compared them to experimental results. We find that the quantum mechanical treatment of the EPC has a crucial impact on the fine structure of the spectra and explains the band features of the experimental spectra for HOMO and LUMO of pentacene.

CPP 37: Focus Session: Interactions Between Water and Cellulose II

Time: Thursday 16:15–17:15 Location: H34

Invited Talk CPP 37.1 Thu 16:15 H34

Modelling Hygroexpansion of Compression and Opposite Wood of Conifer Branches: Bridging the Gap between Molecular and Cell Wall Level — Marie Hartwig-Nair, Sara Florisson, Kristofer Gamstedt, and •Malin Wohlert — Dep of Materials Science and Engineering, Uppsala University

Softwood branches develop compression wood (CW) in the lower and opposite wood (OW) in the upper part exhibiting different hygromechanical properties and differ in structure at several length scales. Distinctive differences are found at cell level, cell wall level and at the level of chemical composition of the lignin and hemicellulose matrix.

The effect each of these respective differences have on tissue level of wood hygromechanical properties is not yet clear. Here, a hierarchical multiscale modelling approach is employed, where the impact composition, MFA and lignin chemical difference have on wood hygroexpansion is studied by the means of hierarchical modelling as support to tissue level experimental investigation of CW and OW hygroexpansion [1]. With atomistic models and Molecular Dynamics simulations of lignin at different levels of hydration, swelling coefficients for the different lignin matrices are obtained [2] and implemented in a Finite Element (FE) model of the cell wall. The FE model also accounted for differences in MFA and composition.

The results of the FE model will be discussed and connected to the MD and tissue level results.

[1] M. Hartwig-Nair et al., Wood Sci. Technol., 2024, 58, 887-906.
[2] M. Hartwig-Nair et al., Wood Sci. Technol., 2024, in press.

CPP 37.2 Thu 16:45 H34

Exploring Hygroexpansion of Cellulose Based Fibers via μCT — •Maximilian Fuchs[1,2], Raimund Teubler[2,3], Alexandra Serebrennikova[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

Understanding the swelling of cellulose-lignin-based fibers is crucial for describing the processes involved in the uptake of water or other volatile organic compounds in paper. Microcomputed tomography (μCT) promises to monitor the hygroexpansion on a paper sheet level. However, extracting and analyzing individual fibers from the interwoven fiber network in these μCT images is challenging. We present a new approach to identify, extract, and analyze hollow fibers by focusing on the fiber lumen as the structural backbone. Using this approach, we quantify changes in fiber shape as the paper sheet absorbs water and another polar solvent, dimethyl sulfoxide (DMSO), from the vapor phase. We continue to observe these changes long after saturation, when no further mass is absorbed in the fibers. With both water and DMSO, the fiber wall thickness continues to increase even after reaching saturation. Furthermore, when exposed to water, the fibers tend to become rounder during swelling, suggesting fiber decollapse. In contrast, the data for DMSO indicates that the outermost fiber layer gets damaged, leading to unrestricted swelling once saturation is exceeded.

CPP 37.3 Thu 17:00 H34

Structure and dynamics of water adsorbed to amorphous cellulose: a comparison of experimental and simulated neutron scattering data — •Veronika Reich[1], Martin Müller[1,2,3], and Sebastian Busch[1] — [1]German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum hereon GmbH, Garching, Germany — [2]Institute of Materials Physics, Helmholtz-Zentrum hereon GmbH, Geesthacht, Germany — [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Kiel

Neutron scattering experiments provide valuable insights into the nanoscopic properties of matter, a scale that is also accessible through Molecular Dynamics (MD) simulations. If the simulations reproduce the experiments, they can give greater insight into the material properties on the nanoscopic scale than traditional data analysis methods. In our work we establish a connection between published experimental data about water absorbed to amorphous cellulose from neutron experiments [1] and MD simulations. Special focus was put on the comparison of the structure factor of non-crystalline water and the dynamics as a function of temperature. The MD simulations were designed to be close to the experimental data from literature to achieve a meaningful comparison.

[1]Czihak, Christoph: Cellulose: Structure and dynamics of a naturally occurring composite material as investigated by inelastic neutron scattering, PhD thesis in material science, University of Vienna (Austria) and Institute Laue-Langevin (France), 2000

CPP 38: Interfaces and Thin Films II

Time: Thursday 16:15–17:45 Location: H38

Invited Talk CPP 38.1 Thu 16:15 H38

Adsorption and Interaction of Amino Acids on Titanium Oxide Photocatalyst — Miguel Blanco-Garcia[1], Mona Kohantorabi[1], Benedikt Socher[2], Ulrike Protzer[3], Stephan V. Roth[2], Cristiana Di Valentin[4], Andreas Stierle[1], and •Heshmat Noei[1] — [1]Centre for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [3]Institute of Virology, Technical University of Munich/Helmholtz Munich, 81675 Munich, Germany — [4]Department of Materials Science, University of Milano-Bicocca, Via R. Cozzi 55, I-20125, Milano, Italy

We investigated the adsorption behavior of amino acids and SARS-CoV-2 virus on rutile (110) and anatase (101) TiO2 surfaces through a combined experimental and theoretical approach and explored the molecular configurations and bonding mechanisms involved in interaction of cysteine and SARS-CoV-2 with TiO2. Clarification of the interaction of the virus with the surface of semiconducting oxides will aid in obtaining a deeper understanding of the chemical processes involved in photo-inactivation of microorganisms which is important for developing advanced photocatalytic materials for environmental and biomedical applications. [1] M. Kohantorabi, et al., ACS Appl. Mater. Interfaces 16, 28 (2024) 37275. [2] M. Kohantorabi, et al., ACS Appl. Mater. Interfaces 15, 6 (2023) 8770.

CPP 38.2 Thu 16:45 H38

PNIPAM Microgel-Stabilized Foam Films: Effect of Crosslinker Content and Purification State — •Luca Mirau, Joanne Zimmer, Kevin Gräff, Matthias Kühnhammer, and Regine von Klitzing — Institute for Condensed Matter Physics, TU Darmstadt, Germany

Aqueous foams find widespread application in fields such as cosmetics, food industry, oil recovery and fire-fighting. Their stabilization requires the presence of surface-active molecules or colloidal particles. In this study, thermoresponsive microgels (MGs) composed of poly(N-isopropylacrylamide) (PNIPAM) with varying crosslinker contents are applied as foam stabilizers, resulting in temperature-sensitive foams. Foam films serve as the fundamental building blocks of foams. The structuring of MGs within these films is analyzed using the Thin Film Pressure Balance (TFPB) technique. Foam films are formed within a pressure chamber, and their thickness is determined through interferometric methods under a light microscope. The foam films display an inhomogeneous structure comprising significant pattern formation, i.e. a network-like, several 100nm thick region containing MGs, interspersed with thin MG-depleted zones less than 100nm thick. The findings indicate that the crosslinking content plays a crucial role in MG layering within these thick network regions, influencing the film thickness. Additionally, the purification state of the MGs, monitored through interfacial tension measurements, governs the formation of thin zones in the foam films, which strongly affects their stability.

CPP 38.3 Thu 17:00 H38

Ion Specific Effects and Photo-Switching of Surfactants at Interfaces — •Dana Glikman and Björn Braunschweig — Institute of Physical Chemistry and Center for Soft Nanoscience, University of Münster, Busso-Peus-Str. 10, 48149 Münster (Germany)

Understanding surface charging and molecular structure changes at oil/water (O/W) interfaces in nanoemulsions is critical for enhancing colloidal properties. In previous work, we demonstrated that photoswitchable surfactants could modulate interfacial behavior. Specifically, we studied an arylazopyrazole (AAP) derivative that undergoes photoisomerization between E and less surface-active Z isomers. In nanoemulsions with droplets showing an average radius of 90 nm, no significant changes in drop size or ζ-potential were observed upon E/Z photo-isomerization. However, second-harmonic scattering (SHS) revealed substantial changes in surfactant coverage which were attributed to ion condensation at the interface [1]. In this contribution, we now focus on the role of specific ion effects and the structural influence of the surfactants' head group. By systematically varying between Li, Na, and Cs cations and by using surfactants with different head group architectures, we aim to dissect the interplay between ionic specificity and head group structure. To study the adsorption of the surfactants at the interface, we are analyzing SHS profiles combined with measurements of the ζ-potential at the shear plane, in order to reveal a detailed mechanisms of ion-specific effects and ion condensation in these nanoemulsions. [1] Glikman et al. J. Am. Chem. Soc. 146, 8362 (2024).

CPP 38.4 Thu 17:15 H38

Anomalous Screening Behavior of Superchaotropic Ions — •Thomas Tilger, Esther Ohnesorge, Michalis Tsintsaris, 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 such as wastewater treatment, separation of nuclear waste and the stabilization of foams, the interest in superchaotropic nano ions grew during the last years. Especially for the last application, it is crucial to understand how the presence of these ions modifies the interaction between interfaces.

To directly measure the forces between well-defined interfaces, colloidal probe atomic force microscopy (CP-AFM) has proven to be a powerful tool. As model system for nano ions we chose Keggin ions as well as dodecaborate clusters and investigated their influence on the interaction between colloidal silica beads in aqueous solutions.

It turned out that - despite the large ion size of up to one nanometer - the interaction between the silica beads can still be described by the classical 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. This might be a hint for an ion aggregation. The magnitude of the deviation depends on the type of nano ion as well as the concentration of the solution.

CPP 38.5 Thu 17:30 H38

The Physics of Water-based Inkjet Printing: Fundamentals in a Nutshell — Helder Savaldor[1,2] and •Nicolae Tomozeiu[1,2] — [1]Canon Production Printing, P.O Box 101, Van der Grintenstraat 1, 5914HH Venlo, The Netherlands — [2]Fluids & Flows Group, Department of Applied Physics, Eindhoven University of Technology, The Netherlands

The printing industry is rapidly evolving, driven by advances in understanding physical-chemical processes and societal needs. Digital inkjet printing, especially with water-based inks, has become a cornerstone of sustainable and cost-effective printing, with Canon Production Printing (CPP) leading innovations in this field. The interaction between ink droplets and porous paper is crucial to achieving high-quality prints, and understanding these processes is essential for improving print performance and durability.

This work explores key scientific domains involved in CPP water-based inkjet technology. We focus on: (i) ink formulation through chemical and polymer physics for optimal droplet formation and film creation; (ii) the dynamics of thin films, including ink spreading, evaporation, and imbibition in porous paper; (iii) surface science's role in ink absorption and spreading. We will show the use of Optical Spectroscopy, Scanning Electron Microscopy (SEM), Nuclear Magnetic Resonance (NMR) and uGISAXS to provide deeper insights into ink film formation at the micro- and nano-level. These findings optimize print quality, durability, and color properties, advancing both industrial development and academic knowledge in inkjet technology.

CPP 39: Members' Assembly

Time: Thursday 18:00–19:00 Location: H38

All members of the Chemical and Polymer Physics Division are invited to participate.

CPP 40: Energy Storage and Batteries II

Time: Friday 9:30–11:15 Location: H34

CPP 40.1 Fri 9:30 H34

Nanoscale Agglomeration Mechanisms of BF-DPB:BPyMPM Donor-Acceptor Systems for Organic Optoelectronic Devices — •Milena Merkel[1], Philipp Wiesener[1], Robert Schmidt[1], Rishi Shivhare[2,3], Rudolf Bratschitsch[1], Saeed Amirjalayer[4], Koen Vandewal[2,3], and Harry Mönig[1] — [1]Physikalisches Institut, Münster University, Münster, Germany — [2]Institute for Materials Research (imo-imomec), Hasselt University, Hasselt, Belgium — [3]imec, imo-imomec, Diepenbeek, Belgium — [4]Interdisciplinary Center for Scientific Computing, Heidelberg University, Heidelberg, Germany

The molecular order of photo-active molecules of organic optoelectronic devices has major impact on their performance. However, it is usually investigated only by indirect measurements or simulations. Here we use low-temperature scanning probe microscopy to image the molecular assembly and interfaces of the donor and acceptor molecules BF-DPB and BPyMPM with submolecular resolution. We illustrate the crucial effect of the substrate and the position of the nitrogen atoms in the BPyMPM molecules on the formation of intermolecular C-H..N hydrogen bonds, metal coordination bonds and corresponding self-assemblies. Using scanning tunneling spectroscopy, we are able to correlate the increasing disorder at the BF-DPB:BPyMPM interface with an increase in the HOMO-LUMO gap of BF-DPB. Photoluminescence measurements on BF-DPB indicate a significant increase in intersystem crossing due to molecule-substrate interactions. Our results provide new insights for a tailored design of active molecules and contact layers for organic optoelectronic devices.

CPP 40.2 Fri 9:45 H34

Multi-layered electrodes for flexible solid-state super capacitors with polymer-based gel electrolyte — •Reyhaneh Bahramian[1,2,3] and Yaser Abdi[3] — [1]Department of Cognitive Sciences, Faculty of Psychology and Education, University of Tehran, Tehran, Iran — [2]Condensed Matter National Laboratory, Institute for Research in Fundamental Sciences, Tehran 19395-5531, Iran — [3]Nanophysics Research Laboratory, Department of Physics, University of Tehran, Tehran 14395-547, Iran

Flexible solid-state supercapacitors are gaining popularity due to their advantages, including flexibility, lightweight design, high power density, rapid charge and discharge rates, broad operating temperature ranges, long cycle life, safety, and ease of fabrication. The use of gel polymer electrolytes enhances ionic conductivity while addressing safety concerns associated with liquid electrolytes.

This research focuses on developing nanocomposite electrodes using Ag-decorated zinc oxide, synthesized through a chemical deposition method on carbon paper, and ferrite applied via a drop-casting technique. The goal is to create electrodes that can operate across a wide voltage range in a non-aqueous electrolyte.

Advanced characterization techniques, such as atomic force microscopy, X-ray diffraction, field emission scanning electron microscopy, and Raman spectroscopy, are employed to analyze the structural properties of the electrodes. The findings reveal an effective specific capacitance of approximately 70 milliFarads per square centimeter.

CPP 40.3 Fri 10:00 H34

Dual-cation pre-intercalated hydrated vanadium oxide achieves 20,000 cycles in aqueous zinc-ion batteries — •Yan Ran and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Aqueous zinc-ion batteries (AZIBs) have broad application prospects in energy storage due to their low cost and high safety. However, cathode materials still face challenges such as low specific capacity and decreased long-cycle performance. In this work, hydrated vanadium oxide with pre-intercalated K and Mn ions (K0.07Mn0.13V2O5*1.47H2O) was synthesized via a one-step hydrothermal method, demonstrating an excellent specific capacity of 524.7 mA h g-1 at 0.1 A g-1, and outstanding stability with 82.47% capacity retention after 20,000 cycles at 5 A g-1. The co-intercalation of dual cations increases the interlayer spacing while stabilizing the material structure, expanding the ion transport channels, and improving both the specific capacity and long-cycle stability. Moreover, the Zn2+/H+ co-intercalation mechanism was confirmed by ex-situ characterization. This work will provide insights for the development of competitive cathodes in high-performance aqueous batteries.

CPP 40.4 Fri 10:15 H34

Temperature-resolved Crystal Structure of Ethylene Carbonate — •Lea Westphal[1,2], Vladislav Kochetov[2], Volodymyr Baran[3], Maxim Avdeev[4,5], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]MLZ, TUM, 85748 Garching, Germany — [3]DESY, 22607 Hamburg, Germany — [4]ANSTO, NSW 2234, Sydney, Australia — [5]School of Chemistry, University of Sydney, NSW 2006, Sydney, Australia

Lithium-ion batteries (LIBs) have been a dominant power source for portable electronics for over three decades and are of interest for applications in electric vehicles and large-scale energy storage systems. Despite significant advancements in LIB design, the main solvents used in the liquid electrolytes, responsible for the charge transfer between the electrodes, have largely remained the same. A key class of these solvents are linear and cyclic carbonates, which, when two or more solvents are combined with lithium salts and additives, exhibit favorable physical/chemical properties. Ethylene carbonate (EC) is a common solvent in commercial batteries due to its high dielectric constant and its ability to form the protective solid-electrolyte interphase (SEI) layer. However, it has to be mixed with other solvents because of its high melting point. Following the determination of EC's crystal structure from single crystals, this study presents temperature dependent Neutron and Synchrotron Powder Diffraction data, studying the sample from 3 K up to its melting point and investigations by Synchrotron Total Scattering and Pair Distribution Function analysis.

CPP 40.5 Fri 10:30 H34

Polymer-nano-tufts: A hairy story of limited conductivity — •Martin Tress, Alaa Yussef Hassan, Nico Junkers, and Wing Kit Or — Peter-Debye-Institute for Soft Matter Research, Leipzig University, Leipzig, Germany

Here we present an approach to study conductivity in small polymer aggregates of as few as ten chains using dielectric spectroscopy [Macromol Chem Phys, 224 (2023) 2200452]. For that, a nano-structured electrode arrangement is combined with several physico-chemical surface modifications to deposit a regular pattern of gold nanoparticles onto which end-functionalized polymer chains are grafted to create tuft-like ensembles of individualized chain aggregates. For polyethylene, pronounced changes in conductivity are observed in tufts compared to bulk with details indicating an alteration of the type of charge transport. This might signal a switch from fast inter-chain ion hopping, dominating in bulk, to slower intra-chain ion hopping in the tufts attributed to the chain configurations and orientation forced by the grafting. Consequently, this could be a more general phenomenon of polymer-solid interfaces that may explain significantly increased electrode polarization and interfacial resistance in ion-conducting polymers, potentially diminishing their performance. Hence, the hypothesis, that bottle-brush architectures could reduce these unwanted effects, was developed. Supported by preliminary results, this might be a step to improve polymeric electrolytes for various fields ranging from solid-state electrolyte batteries to ion-conducting fuel cell membranes.

CPP 40.6 Fri 10:45 H34

Interpretation of the Impedance Signal of Composite Materials using a 3D Electrical Network Model — •Felix Schug[1,2], Sascha Kremer[2,3], Christian Heiliger[1,2], and Janis K. Eckhardt[1,2,3] — [1]Institute for Theoretical Physics, Justus-Liebig-University Giessen, 35392 Giessen, Germany — [2]Center for Materials Research (ZfM), Justus-Liebig-University Giessen, 35392 Giessen, Germany — [3]Institute of Physical Chemistry, Justus-Liebig-University Giessen, 35392 Giessen, Germany

All solid-state batteries (aSSBs) are promising candidates for next-generation energy storage systems, offering high energy and power densities as well as improved device safety compared to the established lithium-ion batteries. Electrochemical impedance spectroscopy (EIS) is one of the key methods to determine charge transport characteristics of the material components in an aSSB. Many of these components are composed of multiple phases, with various transport processes affecting the impedance response signal. Furthermore, the microstructure of the material manifests as a signal within the impedance spectrum. The interpretation of an impedance spectrum is therefore not straightforward, as many signals overlap or are indistinguishable from each other. We therefore employ a microstructure-resolved 3D electrical network to modulate charge transport on microscopic length scales. This approach reveals how microstructure affects the impedance response, as well as the potential and current distributions within a system. It is used to investigate the impedance of composite materials and to develop guidelines for its interpretation.

CPP 40.7 Fri 11:00 H34

Measuring Local Electrochemical Properties with Scanning Probe Microscopy — •Alexander Klasen and Andrea Cerreta — Park Systems Europe GmbH, Mannheim, Germany

Electrochemical (EC) applications, ranging from novel energy storage systems to advanced catalysts, are defined on an ever-decreasing length scale. Investigating these systems requires to map key functional features with sufficient resolution, such as the local structure, electronic properties and electrochemical response. Scanning probe microscopy-based techniques are well established to investigate surface parameters using the physical interaction with a nanometer-sized probe allows studying properties such as the topography, work function, or adhesion at high resolution. One such technique, Scanning Electrochemical Cell microscopy (SECCM), was first introduced by E. Daviddi, P.R. Unwin, et al. and uses a pipette-based SPM approach to probe local EC features. When brought in close proximity to the sample, the electrolyte-filled pipette pipette creates a small electrolyte meniscus between the pipette aperture and the surface of interest . This confined volume of solution constitutes a small electrochemical cell that allows for local measurements of electrochemical characteristics. In this talk, we discuss the basics of SECCM, present recent examples from literature, discuss the limitations of the technique and outline potential pathways to overcome those.

CPP 41: Charged Soft Matter, Polyelectrolytes and Ionic Liquids I

Time: Friday 9:30–11:15 Location: H38

Invited Talk CPP 41.1 Fri 9:30 H38

Simulations of reaction equilibria in macromolecular systems — •Peter Košovan — Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Prague, Czechia

Most molecular simulations are performed assuming a fixed chemical composition, focusing on structural and conformational changes and intermolecular interactions, while neglecting the possible chemical changes which may occur simultaneously. In this lecture, we present an overview of our modeling work, addressing how reversible chemical reactions affect the properties of macromolecular solutions and gels. In particular, we discuss the effect of acid-base equilibria on the net charge of peptides, synthetic polyelectrolytes, polyelectrolyte hydrogels, and proteins. By comparing with experiments, we show that our models can quantitatively predict how this net charge depends on pH of the solution. Next, we show that a change in the pH can trigger attraction between macromolecules, resulting in the formation of condensates, precipitation or gelation. Finally, we show how changes in the pH can be used to control the uptake of charged proteins into coacervates, and how the pH affects the properties of protein solutions during purification processes used by the pharmaceutical industry: dialysis and ultra- or dia-filtration.

CPP 41.2 Fri 10:00 H38

Surface Charged Polymeric Micelles - A Tunable Model System Studied by SANS — Lingsam Tea[1], Luis Willner[1], Christin Waldorf[1], Olga Matsarskaia[2], Ralf Schweins[2], Stephan Förster[1], Lutz Willner[1], and •Jörg Stellbrink[1] — [1]JCNS-1, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Institut Laue-Langevin, 38042 CEDEX 9 Grenoble, France

We investigate surface charged micelles in aqueous solution formed by carboxy terminated n-octacosyl-poly(ethylene oxide) block copolymers, C-PEO5-COOH with 5 the PEO molar mass in kg/mol, by small angle neutron scattering (SANS), zeta-potential measurements and rheology. The -COOH end group was introduced by selective oxidation of the CH_3OH end group of a C-PEO5-OH precursor using Bobbitt's salt. Micellar solutions of different concentrations in the dilute and semidilute range were investigated at pH 2, 6 and 12 to vary ionic strength and the number of effective surface charges Z. Z was further varied by using mixtures of C-PEO5-COOH and C-PEO5-OH at different mixing ratios. SANS measurements reveal that the intramicellar form factor is identical at the different pH-values which implies that the individual micellar structure is unaffected by the number of surface charges. On the contrary, the intermicellar structure factor and the phase behavior show a strong dependence on Z. In particular, we observe a distinct shift of the liquid - fcc crystal phase boundary. A quantitative analysis in terms of a screened Hard Sphere Yukawa potential reveals a very good agreement between experiment and theory.

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CPP 41.3 Fri 10:15 H38

Orientation analysis in polyelectrolyte multilayer and brush coatings by dichroic ATR-FTIR spectroscopy — •Martin Müller, Mirjam Hofmaier, Patricia Flemming, Olga Guskova, Alexander Münch, and Petra Uhlmann — Leibniz-Institut für Polymerforschung Dresden e.V.

Dichroic ATR-FTIR spectroscopic data on two types of thin oriented polyelectrolyte (PEL) coatings relevant for life science are presented. Trapezoidal silicon multiple internal reflection elements, sealed in-situ cell in ATR mirror attachment with polarizer and commercial FTIR spectrometer were used. (i) At first dichroic ATR-FTIR data on thin PEL multilayer (PEM) coatings composed of a-helical poly(L-lysine) and various polyanions (PLL/PA) at unidirectionally texturized silicon substrates are presented. Based on experimental dichroic ratios RATR, the known angles theta between transition dipole moment (TDM) of Amide I and Amide II vibration and a-helix axis (38°, 73°) and on calculated electrical field components Ex,y,z high in-plane y-axial orientation of PEM was identified. (ii) Secondly, thin cationic PEL brushes with three different grafting densities at silicon substrates were characterized by dichroic ATR-FTIR. Using concept of (i) and angle theta between TDM of n(C=O) vibration of PDMAEMA and molecular main axis (69°), which was determined by atomistic simulations, high out-of-plane z-axial orientation was identified. Swelling in water increased the orientation if compared to dry state. Both PEL coating types may be used as bioactive platforms towards proteins and microorganisms.

CPP 41.4 Fri 10:30 H38

Vertical Polyelectrolyte and Site Diffusion of PSS in PSS/PDADMA Multilayers — Annekatrin Sill, •Per-Ole Hilken, and Christiane A. Helm — Institute of Physics, University of Greifswald, Germany

The spontaneous formation of polyelectrolyte multilayers or polyelectrolyte complexes depends on the (inter)diffusion of polyelectrolytes. We investigate the transport of extrinsic sites - charged polyelectrolyte repeat units balanced by counterions - and their relationship to polymer diffusion. We determine the vertical diffusion coefficient D_{PSS} of polystyrene sulfonate (PSS) repeat units in polyelectrolyte multilayer films from poly (diallyldimethylammonium) (PDADMA) and PSS using a quartz crystal microbalance with dissipation (QCM-D) and analyze the observed film growth. Varying the NaCl concentration c_{NaCl} results in $D_{PSS} = 3.2 \cdot 10^{-20}\ \mathrm{m}^2/\mathrm{s} \cdot e^{\alpha \cdot c_{NaCl}}$. As known from the free volume model, the prefactor is constant for each system. For site diffusion, the exponent is also constant ($\alpha \approx 4.9\ \mathrm{M}^{-1}$). For polymer diffusion, however, α increases linearly with M_{PSS}, the molecular weight of PSS. The results for site diffusion quantitatively agree with those of Fares and Schlenoff (JACS (2017) 139; 14656). Polymer diffusion occurs when $M_{PSS} < 65\,\mathrm{kDa}$ (for $M_{PDADMA} = 117\,\mathrm{kDa}$). For these low PSS molecular weights, the diffusion coefficient is $D_{PSS} = B \cdot M_{PSS}^{-\gamma}$. The dependence of B on c_{NaCl} is a power law, while γ increases linearly with c_{NaCl}.

CPP 41.5 Fri 10:45 H38

Understanding the Mechanisms of pH-Sensitive Collapse of Hydrophobic Polymers — •Varun Mandalaparthy and Nico F. A. van der Vegt — Technical University, Darmstadt

The hydrophobic effect is a important contributor to the stability of proteins and may be influenced by many factors including the pH of the solution. To simplify the study of pH effects on proteins, we parameterize biologically motivated titratable monomers which we insert into the sequence of a hydrophobic polymer and study via constant pH molecular dynamics (MD) simulations. We calculate the potential of mean force of the polymer at different pH values and observe that the collapsed state of the polymer is destabilized when the titratable monomer is more charged (high pH for an acid and low pH for a base). Further, the extent of the destabilization is influenced by the position of the titratable monomer along the polymer sequence. The pK_a value of the titratable monomer is also observed to be sensitive to polymer conformation, in agreement with studies of proteins. We further study a zwitterionic polymer with an acidic and a basic monomer in the same sequence which presents a pH-dependent hairpin formation. Our model provides a simplified yet powerful framework to study pH effects on the hydrophobic effect, providing insights into mechanisms governing the behavior of intrinsically disordered proteins (IDPs) and pH-sensitive drug delivery, among other applications.

CPP 41.6 Fri 11:00 H38

Machine learning potentials for redox chemistry in solution — •Redouan El Haouari[1,2], Emir Kocer[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

Machine-Learning Potentials (MLPs), which can offer the accuracy of quantum mechanics at a fraction of the costs, have been applied with great success in atomistic simulations of many systems. Still, most MLPs rely on environment-dependent atomic energies, and are thus unable to distinguish different oxidation states of simple ions in solution. Here, we show for the example of ferrous (Fe2+) and ferric (Fe3+) chloride in aqueous solution that this limitation can be overcome with 4th-Generation High-Dimensional Neural Network Potentials (4G-HDNNPs), in which the local atomic energies are complemented with global charges from a charge equilibration scheme. We find that the iron oxidation states match the total number of chloride ions in the system irrespective of their positions. Furthermore, the model captures charge transfers between ferrous and ferric ions, enabling the general simulation of redox chemistry in solution involving different oxidation states.

CPP 42: Active Matter IV (joint session BP/CPP/DY)

Time: Friday 9:30–13:00 Location: H44

Invited Talk CPP 42.1 Fri 9:30 H44

Wave propagation in systems of active filaments — •Kirsty Y. Wan — Living Systems Institute, University of Exeter, UK

Active hair-like protrusions called cilia are found in many eukaryotes where they produce physiological flows for a variety of functions. Cilia assume a myriad of configurations both external to an organism for the purposes of feeding or swimming motility, but also internally where they mediate mucociliary clearance in vertebrate tissues. Single cilia can propagate large-amplitude non-decaying bending waves, even in the absence of a cell body. These waves assume a variety of stereotyped forms and frequencies, depending on the species. Multiple cilia also interact to produce different types of local and global coordination patterns, including robust metachronal waves. Do these dynamic states of coordination arise spontaneously, or do they require some form of internal control by the cell or animal? We propose new and emerging organisms to address these questions.

CPP 42.2 Fri 10:00 H44

Metabolic activity controls the emergence of coherent flows in microbial suspensions — •Florian Böhme[1], Alexandros Fragkopoulos[1,2], Nicole Drewes[2], and Oliver Bäumchen[1,2] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Photosynthetic microbes have evolved and successfully adapted to the spatio-temporal variations of environmental parameters within their habitat. In the abscence of light, they can still sustain their biological functionality and metabolic activity through aerobic respiration. However, for the soil-dwelling microalga *Chlamydomonas reinhardtii*, their environment may be deprived of both oxygen and light, resulting in a significant reduction of their swimming velocity [1]. Here, we study the effect of motility and cell density of *C. reinhardtii* in a confined system, on the emergence of bioconvection [2]. This collective phenomenon can be reversibly switched by light and arises due to the natural tendency of the bottom-heavy cells to move against gravity. We show that the rate at which the system evolves, as well as the dominant wavelength of the instability can both be directly controlled by the number density of cells. Further, we provide insights on the internal flow fields and density profiles of single bioconvection plumes for different parameters.

[1] A.A. Fragkopoulos et al., *J. R. Soc. Interface* **18**, 20210553 (2021).
[2] A.A. Fragkopoulos et al., *arXiv*:2407.09884 (2024)

CPP 42.3 Fri 10:15 H44

Tumbling *E.coli* in bulk and close to surfaces — •Pierre Martin[1], Tapan Chandra Adhyapak[2], and Holger Stark[1] — [1]Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Indian institute of science education and research (IISER), Tirupati, India

Escherichia coli (*E. coli*) swims by rotating multiple flagella which are connected to the cell body forming a thick bundle. To change direction, *E. coli* performs tumble events by reversing the rotation of one or more flagella. The involved filaments undergo a series of polymorphic transformations, altering both their helicity and handedness. This complex phenomenon involves the interplay of semiflexible filaments and hydrodynamic flow fields.

Here, we have developed a detailed numerical framework to simulate *E. coli*, capturing the full dynamics of flexible flagella, including their polymorphism and their hydrodynamic interactions. The filaments and the cell body are embedded in a viscous fluid, which we model using multi-particle collision dynamics. We analyzed a large number of tumble events, with fixed tumble time or taken from a gamma distribution, exploring the roles of hook and flagellar flexibility as well as flagellar polymorphism. We find that they strongly influence the distribution of tumble angles. Finally, we also show that close to a flat surface the mean tumble angle is strongly shifted to smaller values. This indicates that tumble events may not be recognized, which could give the impression of suppressed tumbling near surfaces.

CPP 42.4 Fri 10:30 H44

***Trypanosoma brucei* (un)chained - effects of confinement on a parasitic microswimmer** — •Hannes Wunderlich[1], Marinus Thein[2], Lucas Brehm[2], Klaus Ersfeld[2], and Matthias Weiss[1] — [1]Experimental Physics I, University of Bayreuth — [2]Laboratory of Molecular Parasitology, University of Bayreuth

Trypanosoma brucei is a parasitic unicellular microswimmer that causes the African sleeping sickness. An active spiral movement of the parasite, mediated by a microtubule-driven flagellum that wraps around the cell body, is mandatory to evade the host's immune system while exploring tissues and blood vessels. In addition, the nematic sub-pellicular micotubule array plays a pivotal role in the elasticity, propulsion, and navigation of the parasite. To study the features and mechanisms behind the cell's motion in such complex environments, we have mimicked spatial confinement in microfluidic devices with different geometries. Our data show that spatial constraints in narrow channels and channel networks can improve cell locomotion of wild-type trypanosomes, supposedly due to the interaction of the elastic cell body and nearby walls. The addition of microtubule-disrupting drugs or the use of mutant strains with altered post-translational modifications of microtubules resulted in significantly altered swimming velocities and marked changes in the intermittent switching between run and tumble phases. Shape analyses of individual cells suggest that microtubules in the sub-pellicular array, the corset that keeps trypanosomes in their native spindle-like shape, are most affected in these cases.

CPP 42.5 Fri 10:45 H44

Micro-swimmer motility in presence of signaling factors — Agniva Datta, Robert Grossmann, and •Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Germany

The navigation of bacteria through aqueous environments, driven by the rotation of helical flagella, has been a significant region of interest in the biophysics community for the last few decades. In this study, we focus on the motility of our model organism, Pseudomonas putida, which exhibits persistent mobile episodes (Active Brownian motion) interrupted by stochastic reorientation events (turns), driven by flagellar self-propulsion, thereby leading to a run-and-turn motility.

Key motility parameters including tumbling rates, run lengths, trajectory persistence (rotational diffusion coefficient), and the characteristics of the self-propulsion force*are hypothesized to depend on the density of quorum-sensing autoinducer molecules, produced by the bacteria themselves as signaling factors. To test this hypothesis, we expose swimming bacteria to aqueous environments with controlled autoinducer concentrations and analyze the resulting changes in motility patterns. Through a combination of experimental data and theoretical modeling, we aim to elucidate the principles of micro-swimmer motility in presence of signaling molecules.

CPP 42.6 Fri 11:00 H44

Collective dynamics of active dumbbells near a circular obstacle — •Chandranshu Tiwari[1] and Sunil Singh[2] — [1]Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India. — [2]Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India.

We present the collective dynamics of active dumbbells in the presence of a static circular obstacle using Brownian dynamics simulation. The active dumbbells aggregate on the surface of a circular obstacle beyond a critical radius, and the aggregate size increases with the activity and the curvature radius. The dense aggregate of active dumbbells displays persistent rotational motion with a certain angular speed, which linearly increases with activity. Furthermore, we show a strong polar ordering of the active dumbbells within the aggregate. The polar ordering exhibits long-range correlation, with the correlation length corresponding to the aggregate size. Additionally, we show that the residence time of an active dumbbell on the obstacle surface increases rapidly with area fraction due to many-body interactions that lead to a slowdown of the rotational diffusion. This article further considers the dynamical behavior of a tracer particle in the solution of active dumbbells. Interestingly, the speed of the passive tracer particle displays a crossover from monotonically decreasing to increasing with the size of the tracer particle upon increasing the dumbbells' speed. Furthermore, the effective diffusion of the tracer particle displays non-monotonic behavior with the area fraction; the initial increase in diffusivity is followed by a decrease for a larger area fraction.

CPP 42.7 Fri 11:15 H44

Free growth under tension — •Chenyun Yao and Jens Elgeti — Forschungszentrum Jülich GmbH, Jülich, Germany

Ever since the ground breaking work of Trepat et al. in 2009, we know that cell colonies growing on a substrate can be under tensile mechanical stress. The origin of tension has so far been attributed to cellular motility forces being oriented outward of the colony. Works in the field mainly revolve around how this orientation of the forces can be explained, ranging from velocity alignment, self-sorting due to self-propulsion, to kenotaxis.

In this work, we demonstrate that tension in growing colonies can also be explained without cellular motility forces! Using a combination of well established tissue growth simulation technique and analytical modelling, we show how tension can arise as a consequence of simple mechanics of growing tissues. Combining these models with a minimalistic motility model shows how colonies can expand while under even larger tension. Furthermore, our results and analytical models provide novel analysis procedures to identify the underlying mechanics.

15 min. break

CPP 42.8 Fri 11:45 H44

A route to active turbulence in circular activity spots — •Arghavan Partovifard and Holger Stark — Institute of Theoretical Physics, Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623Berlin, Germany.

Active nematics exhibit distinctive behavior such as active turbulence and regular flow patterns under spatially varying activity [1]. Utilizing the Doi-Edwards theory supplemented by an active stress tensor [1], we investigate active nematics confined to a circular spot by switching off activity outside the spot. The open boundary allows topological defects to enter and leave the spot.

We calculate the total topological defect charge inside the spot using three approaches: counting all defects, measuring the rotation of the director field along the rim of the spot, and integrating the diffusive charge density. All methods agree that for spot radii just larger than the nematic coherence length, the system has a total topological charge of $+1$, where two $+1/2$ defects perform a regular swirling motion. As the radius increases, more defects enter and their motion becomes more and more chaotic. Ultimately, the charge per unit area saturates at the value characteristic of bulk active turbulence. For the range of radii where the total charge in the spot is $+1$, the nematic director exhibits shear-induced anchoring at an angle of 45° with respect to the tangent at the spot rim. With increasing radius, when more defects enter, the anchoring angle deviates from 45° but its distribution still peaks around this value.

[1] A. Partovifard *et. al.*, Soft Matter **20**, 1800 (2024)

CPP 42.9 Fri 12:00 H44

Cognitive flocks: order-disorder transitions and threat evasion — •Priyanka Iyer[1], Cecilia Soroco[2], and Gerhard Gompper[1] — [1]Forschungszentrum Jülich — [2]University of British Columbia, Canada

Directed self-propulsion is ubiquitous in living organisms. From E.Coli dispersing in biofilms to migrating bird flocks, living organisms are constantly out-of equilibrium. By sensing their environment and adjusting their movement, organisms can exhibit emergent patterns and collective behaviors, such as self-organization in human crowds [1], bird flocks, and fish schools. The Inertial Spin Model (ISM) was introduced to explain the fast and robust propagation of information in bird flocks [2], when only alignment interactions are considered. However, more generally, agents exhibit a variety of interactions like local avoidance, cohesion and threat evasion. We show how such behaviors can be incorporated within the framework of the ISM. It is found that local avoidance introduces emergent noise in the system, triggering an order-disorder transition. Exploring the flock dynamics near this transition reveals a complex interplay between cohesion, alignment, and local avoidance, resulting in diverse behaviors such as pronounced shape and density fluctuations, and diffusive motion of the flock. Lastly, by applying the model to a stationary threat scenario, we analyze flock properties that govern threat information propagation in the flock.

[1] Iyer, P. et al. , Comm. Phys. 7.1 (2024): 379.
[2] Attanasi, A. et al. , Nat. Phys. 10, 691-696, (2014)

CPP 42.10 Fri 12:15 H44

Myosin-independent amoeboid cell motility — •Winfried Schmidt, Alexander Farutin, and Chaouqi Misbah — Univ. Grenoble Alpes, CNRS, LIPhy, F-38000 Grenoble, France

Mammalian cell motility is essential for many physiological and pathological processes, such as the immune system, embryonic development, wound healing, and cancer metastasis. Cells have developed the amoeboid migration mode which allows them to move rapidly in a variety of different environments, including two-dimensional confinement, three-dimensional matrix, and bulk fluids. We introduce a model for an amoeboid cell where the cortex is described as a thin shell along the cell surface. The cell shape evolves due to polymerization of actin filaments and the forces acting on the cortex. We find analytically and numerically that the state of a resting, non-polarized cell can become unstable for sufficiently large actin polymerization velocities, resulting in the spontaneous onset of cell polarity, migration, and dynamical shape changes. Notably, this transition only relies on actin polymerization and does not necessitate molecular motors, such as myosin. These findings yield a deeper understanding of the fundamental mechanisms of cell movement and simultaneously provide a simple mechanism for cell motility in diverse configurations.

CPP 42.11 Fri 12:30 H44

Active membrane deformations of a synthetic cell-mimicking system — Alfredo Sciortino[1], •Dmitry Fedosov[2], Gerhard Gompper[2], and Andreas Bausch[1] — [1]Physik Department, Technische Universität München, Garching bei München, Germany — [2]Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany

Biological cells are fascinating micromachines capable of adapting their shape due to the complex interaction between a deformable membrane and the dynamic activity of the cytoskeleton. We investigate the behavior of an active synthetic cell-mimicking system using simulations and experiments. In simulations, the model consists of a fluid vesicle with a few encapsulated growing filaments. In experiments, giant vesicles contain an active cytoskeletal network composed of microtubules, crosslinkers, and molecular motors. These active vesicles show strong shape fluctuations reminiscent of shape changes of biological cells. We analyze membrane fluctuations and show how the intricate coupling between soft confinement and internal active forces results in fluctuation spectra with distinct spatial and temporal scales, differing significantly from those of passive vesicles. Simulations demonstrate the universality of this behavior, quantifying the impact of correlated activity on the dynamics of membrane deformations. This model makes a step toward quantitative description of shape-morphing artificial and living systems.

CPP 42.12 Fri 12:45 H44

Force Generation by Enhanced Diffusion in Enzyme-Loaded Vesicles — Eike Eberhard, •Ludwig Burger, Cesar Pastrana, Giovanni Giunta, and Ulrich Gerland — Physik komplexer Biosysteme, Technische Universität München, Deutschland

Recent experiments show that the diffusion coefficient of some metabolic enzymes increases with the concentration of their cognate substrate, a phenomenon known as enhanced diffusion. In the presence of substrate gradients, enhanced diffusion induces enzymatic drift, resulting in a non-homogeneous enzyme distribution. In this work, we study the behavior of enzyme-loaded vesicles exposed to external substrate gradients using a combination of computer simulations and analytical modeling. We observe that the spatially inhomogeneous enzyme profiles generated by enhanced diffusion result in a pressure gradient across the vesicle, which leads to macroscopically observable effects, such as deformation and self-propulsion of the vesicle. Our analytical model allows us to characterize dependence of the velocity of propulsion on experimentally tunable parameters. The effects predicted by our work provide an avenue for further validation of enhanced diffusion, and might be leveraged for the design of novel synthetic cargo transporters, such as targeted drug delivery systems.

CPP 43: Droplets, Wetting, Complex Fluids, and Soft Matter (joint session DY/CPP)

Time: Friday 9:30–12:45 Location: H47

Invited Talk CPP 43.1 Fri 9:30 H47
From Cavitation in Soft Matter to Erosion on Hard Matter — •Claus-Dieter Ohl — Institute of Physics, Otto-von-Guericke University, Magdeburg, Germany

Cavitation is the technical term for the formation of empty spaces in a liquid. These unstable voids eventually implode and focus energy on small volumes. Shock wave emission, light emission, erosion, and even nuclear reactions are the consequence of this near singular energy focusing. Here, I will present recent research related to cavitation not only in liquids but also in elastic solids and particularly at the interface of both materials. Singularities developing on the axis of symmetry in non-spherical collapses near boundaries are able to amplify shock waves through self focusing. We think that this mechanism is the primary cause for erosion. In contrast, the non-spherical collapse and shock wave focusing near a tissue allows for the penetration of the tissue with liquid jets at 1000m/s and above. The mechanism at play may be relevant in sports and battle zones, as they could lead to traumatic brain injuries.

CPP 43.2 Fri 10:00 H47
Shape switching and tunable oscillations in adaptive droplets — •Tim Dullweber[1,2], Roman Belousov[1], Camilla Autorino[1,4], Nicoletta Petridou[1], and Anna Erzberger[1,3] — [1]European Molecular Biology Laboratory, Heidelberg, Germany — [2]University Heidelberg, Heidelberg, Germany — [3]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany — [4]Faculty of Biosciences, Heidelberg University, Heidelberg, Germany

Soft materials can undergo irreversible shape changes when driven out of equilibrium. When shape changes are triggered by processes at the surface, geometry-dependent feedback can arise. Motivated by the mechanochemical feedback observed in multicellular systems, we study incompressible droplets that adjust their interfacial tensions in response to shape-dependent signals. We derive a minimal set of equations governing the mesoscopic droplet states, controlled by just two dimensionless feedback parameters. We find that interacting droplets exhibit bistability, symmetry-breaking, excitability and tunable shape oscillations ranging from near-sinusoidal to relaxation-type. We apply our framework to model shape measurements in zebrafish embryos and identify a shape-switching mechanism promoting boundary formation. The underlying critical points reveal novel mechanisms for physical signal processing through shape adaptation in soft active materials, and suggest new modes of self-organization at the collective scale.

CPP 43.3 Fri 10:15 H47
Impact of the history force on the motion of droplets in shaken liquids — •Frederik Gareis and Walter Zimmermann — Theoretical Physics, University of Bayreuth

The Basset-Boussinesq history (BBH) force acts on droplets and solid particles in flows, alongside stationary viscous friction, inertia, and gravitational forces. This force arises from vortex shedding around objects undergoing unsteady acceleration. In this study, we analytically calculate the BBH force for spherical, sedimenting heavy particles in horizontally shaken (periodically accelerated) fluids at low Reynolds numbers and identify the parameter ranges where BBH effects are significant. Our results reveal that BBH can increase particle displacement amplitude by over 60 percent, particularly in the transition region between the low-frequency viscous Stokes regime and the high-frequency inertia-dominated regime. Additionally, we derive a power law for the oscillatory displacement amplitude of a particle around its mean position in a horizontally shaken fluid, facilitating clear experimental identification of BBH effects.

CPP 43.4 Fri 10:30 H47
Bubble Dynamics and Transport in Porous Structures: Insights from Mesoscale Simulations — •Qingguang Xie[1], Othmane Aouane[1], and Jens Harting[1,2] — [1]Forschungszentrum Jülich GmbH, Helmholtz-Institut Erlangen-Nürnberg (IET-2), Erlangen, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Bubble formation, detachment, and transport within porous structures are critical phenomena in various applications, including electrolyzers and chemical reactors. We numerically investigate the dynamics of bubble growth and detachment at a catalytic surface using the lattice Boltzmann method. The departure radius of a bubble, growing with either a pinned or moving contact line, shows good agreement with theoretical predictions. Beyond detachment, we examine the subsequent transport of bubbles through a porous transport layer, systematically evaluating transport efficiency by considering factors such as pressure gradients, reaction rates, and pore wettability. Our findings provide valuable insights for optimizing the design of porous structures, potentially resulting in enhanced performance in electrolyzers and other gas-evolving devices.

CPP 43.5 Fri 10:45 H47
Displacements in thin fluid and elastic films — •Andreas M. Menzel — Otto von Guericke University Magdeburg, Germany

We address the displacements of comparatively small objects in flat thin fluid films under low-Reynolds-number conditions or in flat thin elastic sheets under linear elasticity.
It is well-known that the fundamental solution of the corresponding continuum equations for forced in-plane displacements diverges logarithmically in strictly two-dimensional systems, the so-called Stokes paradox. We provide an illustrative way of interpretation and demonstrate how the divergence cancels under pairwise interactions and confinement [1,2]. Interestingly, logarithmic spatial dependencies prevail under rectangular clamping of elastic membranes [3]. Moreover, the divergence is still present in free-standing sheets of finite thickness, unless they are stabilized, for instance, by substrates [4,5].
We are confident that our analytical results will prove useful in corresponding quantitative experimental evaluations.
[1] S. K. Richter, A. M. Menzel, Phys. Rev. E **105**, 014609 (2022).
[2] T. Lutz, S. K. Richter, A. M. Menzel, Phys. Rev. E **106**, 054609 (2022).
[3] A. R. Sprenger, H. Reinken, T. Richter, A. M. Menzel, EPL (Europhys. Lett.) **147**, 17002 (2024).
[4] T. Lutz, A. M. Menzel, A. Daddi-Moussa-Ider, Phys. Rev. E **109**, 054802 (2024).
[5] A. Daddi-Moussa-Ider, E. Tjhung, T. Richter, A. M. Menzel, J. Phys.: Condens. Matter **36**, 445101 (2024).

CPP 43.6 Fri 11:00 H47
Magnetic dynamics in ferromagnetic liquid crystal emulsions — •Christoph Klopp[1], Hajnalka Nádasi[1], Darja Lisjak[2], and Alexey Eremin[1] — [1]Otto von Guericke University, Institute of Physics, 39106 Magdeburg, Germany — [2]Jozef Stefan Institute, Department for Materials Synthesis, 1000 Ljubljana, Slovenia

We explore magnetic liquid crystal (LC) emulsions for applications as manipulatable chemical sensors in giant cells of Characean algae. Such emulsions can be controlled by magnetic fields and provide targeted drug delivery or sensing [1]. The investigated emulsions consist of a ferromagnetic liquid crystal [2] dispersed in an aqueous solution. We investigate the dynamic magnetic response using AC-susceptometry [3] as a function of the carrier medium viscosity and the particle or droplet size distribution. The emulsions' magnetic spectra differ drastically from those in the bulk of the hybrid liquid crystal mixture. We demonstrate the influence of the liquid crystal director configuration at the water-droplet interface by analyzing the effect of different surfactants (mainly SDS and PVA) in the aqueous phase.
[1] F. von Rüling et al., Liquid Crystals, 2024, 51, 1546
[2] A. Mertelj, et al., Nature, 2013, 504, 237-241
[3] M. Küster et al., J. Magn. Magn. Mater., 2023, 588, 171368
This study was supported by DFG with projects ER 467/14-1 and NA1668/1-3.

15 min. break

CPP 43.7 Fri 11:30 H47
Drying effects in soft colloidal monolayers — •Kai Luca Spanheimer[1], Matthias Karg[2], Nicolas Vogel[3], Liesbeth Janssen[4], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [2]Physikalische Chemie I: Kolloide und Nanooptik Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [3]Lehrstuhl für Partikelsynthese Friedrich-Alexander-Universität,91058 Erlangen,

Germany — [4]Soft Matter and Biological Physics Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

Langmuir-Blodgett deposition is a staple of colloidal monolayer research. It is used in sample preparation for imaging techniques, that spatially resolve colloid patterns. Recent experimental observations have shown that drying can strongly rearrange micron sized microgel patterns after their deposition. The usual dictum that these drying effects do not play a role for colloidal deposition can thus not be held up as a general rule. While capillary effects are well known to be strong at microscopic length scales and play a significant role in drying processes they have been mostly neglected concerning Langmuir-Blodgett deposition. In order to better understand the mechanism of drying we propose a model based on capillary attraction as well as hard core and soft shell repulsion. This model reproduces colloid patterns observed at interfaces as well as ones that occur after drying in the corresponding parameter regimes. From here we are able to derive parameter ranges where drying can play a role in rearranging patterns of colloids and where it can't.

CPP 43.8 Fri 11:45 H47

Interplay of Elasticity and Capillarity in Droplets on Flexible Sheets

— •Salik Sultan and Holger Stark — Technische Universität Berlin, Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Droplets resting on flexible sheets deform into lens-like shapes, offering promising applications in areas like tunable liquid lenses. We have extended and employ our fully three-dimensional Boundary Element Method (BEM) simulation framework [1] to investigate dynamic wetting on thin flexible sheets. Our study focuses on the intricate interplay between the mechanical properties of the sheet and droplet behavior, particularly emphasizing contact angle and droplet shape. By varying the tension and mechanical properties of the sheet, our model demonstrates how we can control and tune the shape of the droplet. Additionally, by introducing stiffness gradients, we aim to explore the potential to steer droplets along the sheet via durotaxis. The versatility of our model suggests potential extensions to other soft material and droplet interactions, such as capillary origami. This work sheds light on the complex interactions between soft substrates and liquid interfaces, leading the way for advancements in material science and interfacial biology.

[1] J. Grawitter and H. Stark, Steering droplets on substrates with plane-wave wettability patterns and deformations, Soft Matter 20, 3161 (2024).

CPP 43.9 Fri 12:00 H47

Cluster quasicrystals composed of ultrasoft particles vs. soft quasicrystals built of colloids with hard cores

— Robert F.B. Weigel and •Michael Schmiedeberg — Theoretical Physics: Lab for Emergent Phenomena, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

We study and compare two different approaches for the stabilization of quasicrystals:

First, we consider a Phase Field Crystal model of complex patterns that self-assemble in systems consisting of ultrasoft colloids. Quasicrystals can be either stabilized by interactions with multiple length scales [1,2] or by preferred binding angles as in patchy colloids [3].

Second, we study a system with patchy colloids with a hard core with a Density Functional Theory. The hard-core is implemented by using a variant of the Fundamental Meassure Theory [4] that probably is the best mean field approach to hard particles.

While the ultrasoft particles assemble in cluster quasicrystals where the particles can completely overlap, in case of hard cores we observe structures that are rather dominated by the tiles that occur on a local level. Our results explain the differences between quasicrystlas that occur in different systems.

[1] Lifshitz, Petrich, PRL 79, 1261 (1997).

[2] Achim et al., PRL 112, 255501 (2014).

[3] Weigel, Schmiedeberg, Modelling Simul. Mater. Sci. Eng. 30, 074003 (2022).

[4] Rosenfeld, PRL 63, 980 (1989).

CPP 43.10 Fri 12:15 H47

Beyond rings and chains: exploring porous crystals and flexible networks with magnetic colloids

— •Carina Karner — Technische Universität Wien

We report on the self-assembly of magnetic colloids engineered with two distinct magnetic patches positioned at their poles, an advancement from traditional Janus particles with a single magnetic dipole. While Janus particles are known to form a variety of superstructures including chains, rings, and close-packed arrangements [1], the two-patch design significantly expands the range of achievable structures. Our simulation study reveals the formation of porous networks with adjustable flexibility, variable pore sizes, and controllable crystalline order. Notably, we observe the formation of a porous Kagome lattice, reminiscent of the experimental Kagome lattice observed colloids with two hydrophobic patches, the well known Janus-triblock system [2]. This enhanced self-assembly behavior in two-patch magnetic particles opens up further possibilities for creating fully tunable, field-responsive ferrofluids. Such systems could useful for applications requiring externally modulated viscosity, such as adaptive damping systems in automotive and aerospace engineering. [1] Vega-Bellido, G. I., DeLaCruz-Araujo, R. A., Kretzschmar, I., & Córdova-Figueroa, U. M. (2019). Self-assembly of magnetic colloids with shifted dipoles. Soft Matter, 15(20), 4078-4086. [2] Chen, Q., Bae, S. C., & Granick, S. (2011). Directed self-assembly of a colloidal kagome lattice.Nature,469(7330), 381-384.

CPP 43.11 Fri 12:30 H47

Effect of geometrical confinement on friction in soft solids

— •Aashna Chawla and Deepak Kumar — Department of Physics, Indian Institute of Technology Delhi, New Delhi 110016, India

Soft and biological materials come in a variety of shapes and geometries. When two soft surfaces with mismatched Gaussian curvatures are forced to fit together, beautiful patterns emerge at the interface due to geometry-induced stress. In this study, we explore the effect of geometrically incompatible confinement of a thin sheet on a soft hydrogel substrate on friction. We use a novel experimental setup to measure the friction between a thin flat elastic sheet placed on a low-friction hydrogel substrate. We show that the frictional force at the interface strongly depends on the geometry and is significantly larger for the geometrically incompatible configuration of a flat sheet on a spherical substrate compared to the other two geometrically compatible configurations: flat sheet on a flat substrate and flat sheet on a cylindrical substrate. Furthermore, for the incompatible configuration of the flat sheet on a spherical substrate, we observe that the frictional force increases monotonically with the sheet radius, with a transition in the behavior at an intermediate radius. We show that these effects arise from the coupling of the stress developed in the sheet due to its geometrically incompatible confinement with the curvature of the interface, resulting in an increased normal force, thereby increasing friction. The insights gained from this study could have significant implications for our understanding of friction in various biological, nanoscale, and other soft systems.

CPP 44: 2D Materials

Time: Friday 11:30–12:30 Location: H34

CPP 44.1 Fri 11:30 H34

Sensors based on graphene field-effect transistors functionalized with molecularly imprinted polymers — •David Kaiser[1], Hamid Rasouli[1], Michael Ringleb[2,3], Ludwig Büttner[2], Martin Hager[2,4], Guobin Jia[5], Jonathan Plentz[5], Christian Beringer[4], Patrick Bräutigam[4], Uwe Hübner[5], Patrick Endres[2], Christof Neumann[1], Steffi Stumpf[2,3], Benjamin Dietzek-Ivanšić[1,4,5], Ulrich S. Schubert[2,3,4] und Andrey Turchanin[1,3,4] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena — [2]Laboratory of Organic and Macromolecular Chemistry, Friedrich Schiller University Jena — [3]Jena Center for Soft Matter, Friedrich Schiller University Jena — [4]Center for Energy and Environmental Chemistry Jena, Friedrich Schiller University Jena — [5]Leibniz Institute of Photonic Technology (Leibniz IPHT)

Monitoring of micropollutants has become a regulatory requirement due to their environmental and health impacts. However, their on-site detection remains challenging, as current methods require transporting samples to centralized laboratories. Here, we present a method for the direct identification of the pharmaceutical carbamazepine (CBZ) utilizing solution-gated graphene field-effect transistors (SG-GFETs) that is appropriate for on-site use. We integrate molecularly imprinted nanoparticles (MIPs) with a diameter of 20 nm onto graphene via their self-assembly, creating highly stable films that specifically bind CBZ, and demonstrate a detection sensitivity reaching as low as 1 pM in buffer solutions and 10 pM in samples of environmental water.

CPP 44.2 Fri 11:45 H34

Efficient DFT Band Gap Correction for 2D-Covalent Organic Frameworks Towards Hybrid Functional Level — •Laura Fuchs and Frank Ortmann — Technische Universität München, TUM School of Natural Sciences

Density functional theory (DFT) is the workhorse computational tool for predicting the structure and physical properties of inorganic and organic molecules as well as semiconductors. Unfortunately, the optical and fundamental band gaps are not well described by semi-local DFT approaches. In particular, common DFT methods like the local density approximation (LDA) and the generalized gradient approximation (GGA) severely underestimate the fundamental band gaps, which is commonly referred to as the "band gap problem". However, the correct band gap is of utmost importance for evaluating the suitability of materials such as organic semiconductors for applications like photocatalysis or green energy harvesting. Besides highly expensive many-body perturbation theory, hybrid functionals can address the band gap problem. However, these functionals still involve high computational costs and, for large two-dimensional covalent organic frameworks (2D-COFs), these efforts are not always feasible. Here, we study the relation between semi-local PBE and hybrid HSE06 functionals and present a simple and computationally cheap scheme to extrapolate the PBE band gaps in 2D-COFs to a more precise band gap at HSE06 level.

CPP 44.3 Fri 12:00 H34

Towards the Computational Design of Molecular Olfactory Receptors for Digital Odor Detection — •Li Chen[1], Leonardo Medrano Sandonas[1], Arezoo Dianat[1], Nina Tverdokhleb[1], Rafael Gutierrez[1], Alexander Croy[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center for Biomaterials, TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena

We present the MORE-Q dataset using quantum-mechanical (QM) simulations for dimer systems composed of body odor volatilome (BOV) and olfactory receptors. The dataset contains abundant QM properties of diverse BOV-receptor systems, both in the gas phase and when deposited on a graphene surface. After analyzing the property space spanned by MORE-Q, we observed flexibility when searching for a dimer configuration with a desired set of electronic binding features. To gain insights into the complex interplay between these sensing properties, an ensemble learning method (XGBoost) was constructed for the fast evaluation of BOV adsorption behavior using only the dimer configurations properties. The results show a significant increase in model performance by adding multiple conformers to the training procedure, and SHAP analysis identifies the most relevant descriptors for predicting the binding features. Our work provides valuable insights into the the sensing mechanism of BOV molecules and paves the way for the computational design of receptors with targeted sensitivity and selectivity.

CPP 44.4 Fri 12:15 H34

Effective EMI shielding solutions: the role of 2D materials and their performance across frequency ranges — •Reyhaneh Bahramian[1,2] and Mohammad Nezafati[2] — [1]Department of Cognitive Sciences, Faculty of Psychology and Education, University of Tehran, Tehran, Iran — [2]Condensed Matter National Laboratory, Institute for Research in Fundamental Sciences, Tehran 19395-5531, Iran

The rise in electronic device usage has led to increased electromagnetic interference (EMI), creating a pressing need for effective shielding materials that are flexible, lightweight, cost-efficient, and high-performing. Two-dimensional (2D) materials are emerging as strong candidates for next-generation EMI shielding solutions. This review examines the origins of electromagnetic responses and shielding mechanisms, focusing on photon-matter interactions, and evaluates the instruments and standards for measuring shielding effectiveness.

Recent advancements in 2D materials for EMI shielding are analyzed, comparing their performance across different frequency ranges with other composite materials. Although 2D material-based composites show significant promise, challenges remain in expanding their applications, particularly in the sub-gigahertz range.

CPP 45: Charged Soft Matter, Polyelectrolytes and Ionic Liquids II

Time: Friday 11:30–12:45 Location: H38

CPP 45.1 Fri 11:30 H38

Binding of small molecules to polyelectrolytes driven by electrostatics — •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden

The interaction of small molecules or ligands to macromolecules (polyelectrolytes or proteins) in solution is plays an important role in biological and medical applications. Pulsed-field-gradient (PFG) nuclear magnetic resonance (NMR) has been applied to measure translational motion of molecules and complexes in aqueous solution, that may be diffusion orelectrophoretic motion. Two-dimensional NMR experiments correlating chemical shift that is used to assign different species with either the diffusion coefficient or the electrophoretic mobility enable determining the mobility of diffusion coefficient respectively in mixtures for the individual components. From the combination of diffusion and electrophoresis NMR the effective charge of the species under investigation is derived. Weak interaction of the ligand to the macromolecule means that the ligand binds for a fraction of time to the macromolecule and is free in the solution for another fraction. From the thus observed weighted average the bound fraction is calculated for every condition no titration experiment is required. The strong polyelectrolyte PDADMAC has been studied interacting with glutamic acid as a function of pH. The bound fraction of glutamic acid increases with increasing pH and thus increasing negative charge of glutamic acid showing that the interaction is driven by electrostatic interaction rather than other possible interactions. The bound fraction as a function of pH coincides with the charge.

CPP 45.2 Fri 11:45 H38

How charge regulation affects adsorption of proteins into polyelectrolyte brushes: A simulation study — •Keerthi Radhakrishnan and Christian Holm — Institute for Computational Physics, University of Stuttgart, D-70569 Stuttgart, Germany

In recent years, polyelectrolyte (PE) brushes have drawn significant attention for their industrial and biomedical applications, particularly their ability to immobilize proteins via electrostatic interactions, even beyond the isoelectric point where both brush and protein share a similar charge. This counterintuitive phenomenon is normally attributed to ”charge patch” effects from protein surface heterogeneity or ”charge regulation” involving reionization and charge reversal near charged entities.

Using coarse-grained simulations, we investigate weak PE brushes interacting with pH-responsive ampholytic nanoparticles exhibiting patchy and non-patchy charge distributions. Building on prior single-ion models, we incorporate realistic protein models with asymmetric charge group distributions to explore higher-order and charge patch-induced effects. Our findings reveal the critical role of charge regulation stemming from anisotropic nanoparticle surface charge, brush potential, and brush-induced pH modulation in driving protein adsorption beyond the isoelectric point.

[1] K. Radhakrishnan, D. Beyer, and C. Holm, How Charge Regulation Affects pH-Responsive Ampholyte Uptake in Weak Polyelectrolyte Brushes, https://doi.org/10.26434/chemrxiv-2024-b10lj-v2., Macromolecules, in print.

CPP 45.3 Fri 12:00 H38

Molecular Dynamics Simulations of Structural and Dynamical Properties of Polymerized Ionic Liquids — •Arshid Ahmad and Michael Vogel — Institute for Condensed Matter Physics, Technische Universität Darmstadt, Darmstadt, Germany

Ionic liquids consist of cations and anions and have melting points less than 100°C. Their key features include negligible vapor pressure, high thermal stability, and favorable solvation properties, rendering them valuable materials for applications, e.g., in green chemistry and electrochemistry. In addition to these simple ionic liquids (SILs), polymerized ionic liquids (PILs) receive considerable attention because they add the favorable mechanical properties of polymers to these systems. We present MD simulations of a SIL and a corresponding PIL. The latter comprises BF4 anions and polymerized cations, which feature imidazolium rings connected by 6 methylene groups along the backbone. We use MD simulations to determine both structural and dynamical properties of this PIL. In particular, we relate the temperature-dependent local and diffusive dynamics of the anions and polymerized cations and we analyze dynamical couplings of both components. For the anions, the analysis includes the mechanism and f the motion. For the polymerized cations, we investigate not only the segmental motion but we also tackle the question to which degree the Rouse model is capable of describing the dynamics of highly charged polymer chains, which strongly interact with counter-ions. A detailed comparison of the results for the SIL and PIL reveals the effects of cation polymerization on structural and dynamical properties.

CPP 45.4 Fri 12:15 H38

Condensate size control by charge asymmetry — •Chengjie Luo[1], Nathaniel Hess[2], Dilimulati Aierken[2], Yicheng Qiang[1], Jerelle A. Joseph[2], and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization — [2]Princeton University

Biomolecular condensates are complex droplets composed of various types of biomolecules, including nucleic acids and proteins. These condensates form mainly due to liquid-liquid phase separation, which is driven by short-range attraction between biomolecules. Typical biomolecules carry various net charges, so that long-ranged electrostatic interactions could affect phase separation. We study this situation using a simple model of two short-ranged attractive polymers with opposite charges and their counterions. We find that the charged polymers segregate from the solvent, and thus form two macrophases, when their charges are symmetric. In contrast, many droplets of equal size coexist when charge asymmetry is sufficiently strong. Such patterned phases form because the short-range attraction concentrates polymers within droplets, leading to net charges, which prevents droplet growth. Our molecular dynamics simulation and a continuous field theory demonstrate that droplet size decreases with charge asymmetry. Overall, we present a mechanism controlling droplet size via a trade-off between short-ranged attraction driving phase separation and long-ranged electrostatic repulsion if droplets accumulate net charges. Our results are relevant for understanding biomolecular condensates and creating synthetic patterns in chemical engineering.

CPP 45.5 Fri 12:30 H38

Structural transitions of a Semi-Flexible Polyampholyte — •Rakesh Palariya and Sunil P Singh — Indian Institute Of Science Education and Research, Bhopal , India

Polyampholytes (PA) are charged polymers composed of positively and negatively charged monomers. The sequence of the charged monomers and the bending of the chain significantly influence the conformation and dynamical behavior of the PA. Using coarse-grained molecular dynamics simulations, we comprehensively study the structural and dynamical properties of flexible and semi-flexible PA's. The simulation results demonstrate a flexible PA chain, displaying a transition from a coil to a globule in the parameter space of the charge sequence. Additionally, the behavior of the mean-square displacement (MSD), denoted as $<(\Delta r(t))^2>$, reveals distinct dynamics, specifically for the alternating and charge-segregated sequences. The MSD follows a power-law behavior, where $<(\Delta r(t))^2>\sim t^\beta$, with $\beta \approx 3/5$ and $\beta \approx 1/2$ for the alternating sequence and charge-segregated sequence in the absence of hydrodynamic interactions, respectively. However, when hydrodynamic interactions are incorporated, the exponent β shifts to approximately 3/5 for the charge-segregated sequence and 2/3 for the well-mixed alternating sequence. For a semi-flexible PA chain, varying the bending rigidity and electrostatic interaction strength (Γ_e) leads to distinct, fascinating conformational states, including globule, bundle, and torus-like conformations. The transition between various conformations is identified in terms of the shape factor estimated from the ratios of eigenvalues of the gyration tensor.

CPP 46: Closing Talk (joint session BP/CPP/DY)

Time: Friday 13:15–14:00 Location: H2

Invited Talk CPP 46.1 Fri 13:15 H2

Active control of forces, movement and shape: from biological to non-living systems — •Ulrich S. Schwarz — Heidelberg University, Heidelberg, Germany

Animal cells are highly dynamic and continuously generate force, for example for division, migration and mechanosensing. Their main force generators are myosin II molecular motors, whose activity is precisely controlled by biochemical circuitry. We first discuss how this system can be hijacked by optogenetics, thus that cellular force generation can be controlled in time and space using light. Next, we use active gel theory combined with van der Waals theory for myosin II molecules to demonstrate that cell contractility is sufficient to explain cell migration and that optogenetics can be used to initiate and revert migration. For two myosin II species, we predict the possibility of oscillations. We then move up in scale and analyze force generation in intestinal organoids, which are epithelia with the topology of a sphere. Combining experimental data, image processing and the bubbly vertex model, we show how apico-basal asymmetries can lead to cell extrusion and budding. We finally discuss how force generation and shape changes can be achieved in non-living systems, in particular for nematic elastomers, in which the direction of contraction is imprinted during polymerization and actuation is achieved by temperature control.