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

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The 2026 Meeting of the CPP Division is marked by the 75th anniversary of the Polymer Physics Division, which is celebrated in the Focus Session “75 Years Division Polymer Physics: From Curiosity to Smart Materials”. Two Focus Sessions address the topics “Theoretical Modeling and Simulation of Biomolecular Condensates” and “Water: From Atmosphere to Space”. To honor the guest country France, we have organized the following French-German sessions: “Membranes and Porous Materials”, “Nanomaterials, Composites and Hybrids”, “Simulation Methods and Modeling of Soft Matter”, “2D Materials, Thin Films and Interfaces” as well as a Round Table Discussion “The Future of Neutrons in France and Germany”. Plenary speakers include Peter Müller-Buschbaum, Hugues Chaté, Antony Hyman, and Annabella Selloni. The former chairman of the CPP Division, Kurt Kremer, is this year’s awardee of the Max Planck Medal. The CPP Division supports the Symposia “The Sustainability Challenge: A Decade of Transformation” and “Fluids with Broken Time-Reversal Symmetry: Odd/Hall Viscosity between Active Matter and Electron Flows” as well as the French-German Symposium “Soft, Active and Alive: Emergent Properties in Living Matter”. The Meeting concludes with a Highlighted Invited Talk given by Jens-Uwe Sommer.

Overview of Invited Talks and Sessions

(Lecture halls ZEU/LICH, ZEU/0255, ZEU/0260, and HÜL/S386; Poster P5)

Invited Talks

CPP 3.1	Mon	9:30–10:00	ZEU/LICH	**Theory and Modeling of Fluid Adsorption and Transport in Nanoporous Materials** — •Benoit Coasne
CPP 4.1	Mon	9:30–10:00	ZEU/0255	**Exploration of Cathode Materials for Li-S Batteries** — •Yan Lu
CPP 5.1	Mon	9:30–10:00	ZEU/0260	**Cleaning of dusty surfaces** — •Doris Vollmer, Franziska Sabath, Abhinav Naga, Stefanie Kirschner, Tarik Karakaya, Rüdiger Berger, Hans-Jürgen Butt, Halim Kusumaatmaja
CPP 6.1	Mon	11:15–11:45	ZEU/LICH	**Hierarchical Porosity Meets Nanoconfined Water: Toward Water-Driven Functional Materials** — •Patrick Huber
CPP 9.1	Mon	15:00–15:30	ZEU/LICH	**Why Polymers Swell or Collapse: Molecular Insights into Cosolute Effects** — •Nico van der Vegt
CPP 12.1	Mon	15:00–15:30	ZEU/0255	**Multifunctional films by tailoring chemistry and morphology of polymer brushes at the nanoscale** — •Petra Uhlmann, Alexander S. Münch
CPP 12.6	Mon	16:30–17:00	ZEU/0255	**Thin-film and interface properties in energy conversion devices unveiled by X-rays** — •Marcus Bär
CPP 13.1	Mon	15:00–15:30	ZEU/0260	**Modelling and simulation of pH-sensitive polyelectrolyte microgels** — •Stefanie Schneider
CPP 16.1	Mon	17:15–17:45	ZEU/0260	**Understanding the Passivation Properties of Solid Electrolyte Interphases (SEIs) in Batteries: Generator-Collector Experiments combined with a Transport and Reaction Model** — •Bernhard Roling, Falk Krauss, Annalena Duncker, Isabel Pantenburg
CPP 21.1	Tue	9:30–10:00	ZEU/0255	**Molecular modelling of gas solubility and free volume trends in Si-functionalized ionic liquids** — •Kateryna Goloviznina, Eduards Bakis, Inês C. M. Vaz, Agilio Padua, Margarida Costa Gomes

CPP 22.1	Tue	9:30–10:00	ZEU/0260	**From Solution to Thin Films: Structure Formation Pathways in Organic Photovoltaic Films** — •Eva M. Herzig
CPP 26.1	Tue	14:00–14:30	HÜL/S386	**Investigating lignin graphitisation depending on botanical source and extraction method** — Lucie Dieval, Phuthiphong Ouitrakoon, Robert Hunter, Sébastien Schaefer, Louis Hennet, Erik Elkaim, Julie Ruellou, Milo S. P. Shaffer, Agnieszka Brandt-Talbot, •Pascale Launois
CPP 30.1	Tue	14:00–14:30	ZEU/0260	**Solvent effects on amphiphile self-assembly in Deep Eutectic Solvents** — •Karen Edler
CPP 31.1	Wed	9:30–10:00	ZEU/0255	**Hydrogels with a Pinch of Embodied Intelligence** — •Andreas Walther
CPP 33.1	Wed	10:00–10:30	ZEU/LICH	**Shape-induced superstructure formation in concentrated ferrofluids** — •Sabrina Disch
CPP 37.1	Wed	15:00–15:30	ZEU/LICH	**Predicting molecular ordering in deposited molecular films** — •Denis Adrienko
CPP 38.1	Wed	15:00–15:30	ZEU/0255	**Engineering, processing and application of recombinant spider silk proteins** — •Thomas Scheibel
CPP 39.1	Wed	15:00–15:30	ZEU/0260	**A polarizable model for atomistic simulations of metals and graphitic material/ liquid interfaces** — Krishan Kanhaiya, Hendrik Heinz, •Marialore Sulpizi
CPP 42.1	Wed	17:00–17:30	ZEU/0260	**Mesopores filled with (poly)ionic liquids: phase transitions under confinement, and structure seen by SAXS and SANS** — •Julian Oberdisse, Anne-Caroline Genix
CPP 44.1	Thu	9:30–10:00	ZEU/LICH	**Shedding light on wide bandgap perovskites** — •Michael Saliba
CPP 53.1	Fri	9:30–10:00	ZEU/LICH	**Limits and Prospects of Organic Solar Cells** — •Dieter Neher
CPP 54.1	Fri	9:30–10:00	ZEU/0255	**NMR-based molecular rheology and structural characterization of model gels** — •Kay Saalwächter, Bidit Lamsal
CPP 56.1	Fri	10:45–11:15	HÜL/S386	**Liquid Dynamics at Interfaces** — •Michael Vogel
CPP 61.1	Fri	13:15–14:00	HSZ/0002	**Biomolecular Condensates: Challenges for Polymer Physics** — •Jens-Uwe Sommer

Topical Talks

CPP 19.1	Tue	9:30–10:00	ZEU/LICH	**Surface adsorption and protonation equilibrium of atmospheric organics at the aqueous surface** — •Nønne Prisle
CPP 27.1	Tue	14:00–14:30	ZEU/LICH	**Why water in plants survives negative pressure** — Marin Šako, Emanuel Schneck, Roland Netz, •Matej Kanduč
CPP 32.1	Wed	9:30–10:00	ZEU/0260	**Synchrotron X-Ray Studies on Structural Transitions in Water and Alcohol containing Ice Analogues** — •Christina M. Tonauer
CPP 45.1	Thu	9:30–10:00	ZEU/0260	**Wetting transitions in biomolecular coacervates** — •Susanne Liese, Tiemei Lu, Evan Spruijt, Christoph Weber
CPP 51.1	Thu	15:15–15:45	ZEU/LICH	**The Loops of Life** — Brian Chan, •Michael Rubinstein
CPP 51.2	Thu	15:45–16:15	ZEU/LICH	**Polyelectrolytes and Biological Systems: A Charged Relationship** — •Matthias Ballauff
CPP 51.3	Thu	16:15–16:45	ZEU/LICH	**From block copolymer morphologies to functional polymer membranes** — •Volker Abetz
CPP 51.4	Thu	16:45–17:15	ZEU/LICH	**Molecular electronic materials and devices for solar energy conversion** — •Jenny Nelson
CPP 51.5	Thu	17:15–17:45	ZEU/LICH	**Control of cell and tissue stiffness by biopolymer networks and particle inclusions** — •Paul Janmey
CPP 55.1	Fri	9:30–10:00	ZEU/0260	**Data-driven modelling of phase-separating intrinsically disordered regions** — •Giulio Tesei, Fatima Kamal Zaidi, Shanlong Li, Julian O. Streit, Jianhan Chen, Tanja Mittag, Kresten Lindorff-Larsen

Discussion on Sustainability on Monday during Lunch Break

PSV I	Mon	13:00–13:45	HSZ/AUDI	**Sustainability! And now? – Opportunities for young researchers** — •Roxana Scharpegge, Hiroki Sayama, Thomas Schubatzky, Birte Höcker, Uwe Riedel, John Plane, Pauleo Nimtz, Stefanie Falk

Invited Talks of the joint Symposium SKM Dissertation Prize 2026 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium The Sustainability Challenge: A Decade of Transformation (SYSC)

See SYSC for the full program of the symposium.

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky
SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Invited Talks of the joint Symposium Fluids with Broken Time-Reversal Symmetry: Odd/Hall Viscosity between Active Matter and Electron Flows (SYBS)

See SYBS for the full program of the symposium.

SYBS 1.1	Tue	9:30–10:00	HSZ/AUDI	**Odd viscosity in three-dimensional fluids: flows, wakes, and eddies** — •Tali Khain
SYBS 1.2	Tue	10:00–10:30	HSZ/AUDI	**Odd viscosity in two-dimensional hydrodynamic electron transport** — •Igor Gornyi, Dmitry Polyakov
SYBS 1.3	Tue	10:30–11:00	HSZ/AUDI	**Odd slip on chiral active surfaces** — •Andrej Vilfan, Yuto Hosaka
SYBS 1.4	Tue	11:15–11:30	HSZ/AUDI	**Parity-odd transport in electron fluids** — •Johanna Erdmenger
SYBS 1.5	Tue	11:30–11:45	HSZ/AUDI	**Curved Odd Elasticity** — Lazaros Tsaloukidis, Yuan Zhou, Jack Binysh, Nikta Fakhri, Corentin Coulais, •Piotr Surówka

Invited Talks of the joint Symposium France: Soft, Active and Alive: Emergent Properties in Living Matter (SYGF)

See SYGF for the full program of the symposium.

SYGF 1.1	Wed	15:00–15:30	HSZ/AUDI	**Liquid crystal geometries in type I collagen-based tissues** — •Nadine Nassif
SYGF 1.2	Wed	15:30–16:00	HSZ/AUDI	**Self-organization of the cytoplasm by physical instabilities** — •Jan Brugues
SYGF 1.3	Wed	16:00–16:30	HSZ/AUDI	**From morphogenesis to space partitioning by microtubules and molecular motors.** — •Manuel Thery

SYGF 1.4	Wed	16:45–17:15	HSZ/AUDI	**More than the sum: how composite interfaces govern function** — •Alba Diz-Muñoz
SYGF 1.5	Wed	17:15–17:45	HSZ/AUDI	**Swimming and Swarming of Intelligent Active Particles** — Segun Goh, Priyanka Iyer, Rajendra Singh Negi, •Gerhard Gompper
SYGF 1.6	Wed	17:45–18:15	HSZ/AUDI	**Perturbing the collective motion of fish with challenging environments** — •Aurélie Dupont

Sessions

CPP 1.1–1.11	Mon	9:30–12:45	BAR/SCHÖ	**Active Matter I (joint session BP/CPP/DY)**
CPP 2.1–2.4	Mon	9:30–10:30	MER/0002	**Sustainability: Challenges and Solutions (joint session UP/CPP/SOE)**
CPP 3.1–3.5	Mon	9:30–11:00	ZEU/LICH	**French-German Session: Membranes and Porous Materials I**
CPP 4.1–4.6	Mon	9:30–11:15	ZEU/0255	**Energy Storage Materials and Devices I**
CPP 5.1–5.5	Mon	9:30–11:00	ZEU/0260	**Wetting, Fluidics and Liquids at Interfaces and Surfaces I (joint session CPP/DY)**
CPP 6.1–6.5	Mon	11:15–12:45	ZEU/LICH	**French-German Session: Membranes and Porous Materials II**
CPP 7.1–7.5	Mon	11:30–12:45	ZEU/0255	**Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods I**
CPP 8.1–8.5	Mon	11:30–12:45	ZEU/0260	**Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)**
CPP 9.1–9.7	Mon	15:00–17:00	ZEU/LICH	**French-German Session: Simulation Methods and Modeling of Soft Matter I**
CPP 10.1–10.13	Mon	15:00–18:30	ZEU/0118	**Droplets, Wetting, and Microfluidics (joint session DY/CPP)**
CPP 11.1–11.12	Mon	15:00–18:30	ZEU/0160	**Active Matter II (joint session DY/BP/CPP)**
CPP 12.1–12.6	Mon	15:00–17:00	ZEU/0255	**French-German Session: 2D Materials, Thin Films and Interfaces I**
CPP 13.1–13.7	Mon	15:00–17:00	ZEU/0260	**Charged Soft Matter, Polyelectrolytes and Ionic Liquids**
CPP 14.1–14.7	Mon	17:15–19:00	ZEU/LICH	**French-German Session: Simulation Methods and Modeling of Soft Matter II**
CPP 15.1–15.7	Mon	17:15–19:00	ZEU/0255	**Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods II**
CPP 16.1–16.6	Mon	17:15–19:00	ZEU/0260	**Energy Storage Materials and Devices II**
CPP 17.1–17.51	Mon	19:00–21:00	P5	**Poster I**
CPP 18.1–18.12	Tue	9:30–12:45	BAR/SCHÖ	**Active Matter III (joint session BP/CPP/DY)**
CPP 19.1–19.5	Tue	9:30–11:00	ZEU/LICH	**Focus Session: Water – from Atmosphere to Space I (joint session CPP/DY)**
CPP 20.1–20.12	Tue	9:30–12:45	ZEU/0160	**Complex Fluids and Soft Matter (joint session DY/CPP)**
CPP 21.1–21.6	Tue	9:30–11:15	ZEU/0255	**French-German Session: Simulation Methods and Modeling of Soft Matter III**
CPP 22.1–22.6	Tue	9:30–11:15	ZEU/0260	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics I**
CPP 23.1–23.6	Tue	11:15–12:45	ZEU/LICH	**Focus Session: Water – from Atmosphere to Space II (joint session CPP/DY)**
CPP 24.1–24.5	Tue	11:30–12:45	ZEU/0255	**French-German Session: Simulation Methods and Modeling of Soft Matter IV**
CPP 25.1–25.5	Tue	11:30–12:45	ZEU/0260	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics II**
CPP 26.1–26.5	Tue	14:00–15:30	HÜL/S386	**French-German Session: 2D Materials, Thin Films and Interfaces II**
CPP 27.1–27.5	Tue	14:00–15:30	ZEU/LICH	**Focus Session: Water – from Atmosphere to Space III (joint session CPP/DY)**
CPP 28.1–28.5	Tue	14:00–15:30	ZEU/0160	**Active Matter IV (joint session DY/BP/CPP)**
CPP 29.1–29.6	Tue	14:00–15:30	ZEU/0255	**Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods III**
CPP 30.1–30.5	Tue	14:00–15:30	ZEU/0260	**Complex Fluids, Colloids, Micelles and Vesicles I**
CPP 31.1–31.7	Wed	9:30–11:30	ZEU/0255	**Responsive and Adaptive Systems**

CPP 32.1–32.4	Wed	9:30–10:45	ZEU/0260	**Focus Session: Water – from Atmosphere to Space IV (joint session CPP/DY)**
CPP 33.1–33.4	Wed	10:00–11:15	ZEU/LICH	**Complex Fluids, Colloids, Micelles and Vesicles II**
CPP 34.1–34.4	Wed	11:00–12:00	ZEU/0260	**Focus Session: Water – from Atmosphere to Space V (joint session CPP/DY)**
CPP 35.1–35.5	Wed	11:15–12:45	ZEU/0118	**Glasses and Glass Transition (joint session DY/CPP)**
CPP 36.1–36.1	Wed	11:45–12:45	ZEU/LICH	**Round Table Discussion: The Future of Neutrons in France and Germany (joint session CPP/BP)**
CPP 37.1–37.6	Wed	15:00–16:45	ZEU/LICH	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics III**
CPP 38.1–38.6	Wed	15:00–16:45	ZEU/0255	**Biopolymers, Biomaterials and Bioinspired Functional Materials I (joint session CPP/BP)**
CPP 39.1–39.6	Wed	15:00–16:45	ZEU/0260	**French-German Session: Nanomaterials, Composites and Hybrids I**
CPP 40.1–40.6	Wed	17:00–18:30	ZEU/LICH	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics IV**
CPP 41.1–41.7	Wed	17:00–18:45	ZEU/0255	**Biopolymers, Biomaterials and Bioinspired Functional Materials II (joint session CPP/BP)**
CPP 42.1–42.6	Wed	17:00–18:45	ZEU/0260	**French-German Session: Nanomaterials, Composites and Hybrids II**
CPP 43.1–43.11	Thu	9:30–12:45	BAR/SCHÖ	**Biomaterials and Biopolymers (joint session BP/CPP)**
CPP 44.1–44.6	Thu	9:30–11:15	ZEU/LICH	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics V**
CPP 45.1–45.6	Thu	9:30–11:15	ZEU/0260	**Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates I (joint session CPP/BP)**
CPP 46.1–46.66	Thu	9:30–11:30	P5	**Poster II**
CPP 47.1–47.7	Thu	10:15–12:45	BAR/0106	**Focus Session: Controlling Microparticles and Biological Cells by Ultrasound (joint session BP/CPP/DY)**
CPP 48.1–48.5	Thu	11:30–12:45	ZEU/LICH	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VI**
CPP 49.1–49.5	Thu	11:30–12:45	ZEU/0255	**Gels, Polymer Networks and Elastomers I**
CPP 50.1–50.5	Thu	11:30–12:45	ZEU/0260	**Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates II (joint session CPP/BP)**
CPP 51.1–51.5	Thu	15:15–17:45	ZEU/LICH	**Focus Session: 75 Years Polymer Physics Division: From Curiosity to Smart Materials (joint session CPP/BP)**
CPP 52	Thu	18:00–19:00	ZEU/LICH	**Members' Assembly**
CPP 53.1–53.6	Fri	9:30–11:15	ZEU/LICH	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VII**
CPP 54.1–54.6	Fri	9:30–11:15	ZEU/0255	**Gels, Polymer Networks and Elastomers II**
CPP 55.1–55.6	Fri	9:30–11:15	ZEU/0260	**Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates III (joint session CPP/BP)**
CPP 56.1–56.4	Fri	10:45–12:00	HÜL/S386	**Molecular and Polymer Dynamics, Friction and Rheology I**
CPP 57.1–57.6	Fri	11:30–13:00	ZEU/LICH	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VIII**
CPP 58.1–58.6	Fri	11:30–13:00	ZEU/0255	**Gels, Polymer Networks and Elastomers III**
CPP 59.1–59.6	Fri	11:30–13:00	ZEU/0260	**Crystallization**
CPP 60.1–60.3	Fri	12:15–13:00	HÜL/S386	**Molecular and Polymer Dynamics, Friction and Rheology II**
CPP 61.1–61.1	Fri	13:15–14:00	HSZ/0002	**Closing Talk (joint session CPP/BP/DY)**

Members' Assembly of the Chemical and Polymer Physics Division

Thursday 18:00–19:00 Raum ZEU/LICH

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

CPP 1: Active Matter I (joint session BP/CPP/DY)

Time: Monday 9:30–12:45 Location: BAR/SCHÖ

CPP 1.1 Mon 9:30 BAR/SCHÖ

Bayesian inference of magnetosensing in a magnetotactic bacterium — •Sascha Lambert[1], Emilie Gachon[2], Damien Faivre[2], and Stefan Klumpp[1] — [1]University of Göttingen, Institute for the Dynamics of Complex Systems, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany. — [2]Aix Marseille Université, CEA, CNRS, BIAM, 13115 Saint-Paul-Lez-Durance, France.

Magnetotactic bacteria are often assumed to align only passively with external magnetic fields, yet recent observations of the magnetotactic bacterium SS-5 reveal a pronounced increase in swimming speed under geomagnetic conditions. Because flagellated microorganisms typically follow helical paths, magnetic torques could, in principle, straighten their trajectories and create an apparent increase in speed, offering a purely mechanical explanation. We test this hypothesis using a physical swimming model based on Active Brownian Particles that incorporates magnetic torques, rotational propulsion, and helical motion, and we explore the relevant parameter space using Bayesian inference constrained by three-dimensional trajectory data. Posterior predictive simulations demonstrate that the mechanically induced increase in apparent speed is far too small to account for the experimental observations, even under extreme parameter choices. The results quantitatively rule out swaying as a sufficient explanation for the behaviour of SS-5 and instead support the presence of an active magnetic sensing mechanism.

CPP 1.2 Mon 9:45 BAR/SCHÖ

Vorticity-induced surfing and trapping in porous media — •Pallabi Das[1], Mirko Residori[1], Axel Voigt[2,3,4], Suvendu Mandal[5], and Christina Kurzthaler[1,3,4] — [1]Max Planck Institute for the Physics of Complex Systems, Germany — [2]Institute of Scientific Computing, TU Dresden, Germany — [3]Center for Systems Biology Dresden, Germany — [4]Cluster of Excellence, Physics of Life, TU Dresden, Germany — [5]TU Darmstadt, Germany

Microorganisms often encounter strong confinement and complex hydrodynamic flows while navigating their habitats. Combining finite-element methods and stochastic simulations, we study the interplay of active transport and heterogeneous flows in dense porous channels. We find that swimming always slows down the traversal of agents across the channel, giving rise to robust power-law tails of their exit-time distributions. These exit-time distributions collapse onto a universal master curve with a scaling exponent of $\approx 3/2$ across a wide range of packing fractions and motility parameters, which can be rationalized by a scaling relation. We further identify a new motility pattern where agents alternate between *trapping* along fast streams and extended *surfing* phases, the latter determining the power-law exponent. Unexpectedly, trapping occurs in the flow backbone itself – not only at obstacle boundaries – due to vorticity-induced reorientation in the highly-heterogeneous flow environment. These findings provide a fundamentally new active transport mechanism with direct implications for biofilm clogging and the design of novel microrobots capable of operating in heterogeneous media.

CPP 1.3 Mon 10:00 BAR/SCHÖ

Adhesion Patterns in Gliding Filamentous Cyanobacteria — •Elias Fischer[1], Paul Nieschwitz[2], Stefan Karpitschka[2], and Holger Stark[1] — [1]Institute of Physics and Astronomy, TU Berlin, Germany — [2]Department of Physics, Universität Konstanz, Germany

Filamentous cyanobacteria play an important role in many ecosystems and the carbon cycle of our planet. They 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.

Our recent measurements of filamentous cyanobacteria gliding across flat surfaces and visualized in kymographs show spatio-temporal adhesion regions along the filament, indicating an intrinsic helical shape. Based on our a novel approach for modeling the mechanical aspects of individual cyanobacteria filaments, we are able to interpret the complex kymograph patterns. Each filament is modeled as a helical chain of thin cylindrical segments in 3D with bending and twisting elasticity. The filaments interact with nearby surfaces and filaments via a hard-core repulsion and an exponentially decaying adhesion force. Importantly, the propulsion forces that push the filament forward are only applied locally at surface-contacting segments.

Our simulated kymographs reveal how both the helical shape and the adhesion strength strongly influence the filament's gliding speed and the dynamics of the surface-attachment regions. Thereby, we crucially contribute to the understanding of how real filamentous cyanobacteria generate their propulsion forces.

CPP 1.4 Mon 10:15 BAR/SCHÖ

The 3D chirality of malaria parasites determines their motion patterns in 2D and originates at the apical pole — •Leon Lettermann[1], Mirko Singer[2], Smilla Steinbrück[2,3], Falko Ziebert[1], Sachie Kanatani[3], Photini Sinnis[3], Friedrich Frischknecht[2], and Ulrich Schwarz[1] — [1]Institute for Theoretical Physics & BioQuant, Heidelberg University — [2]Parasitology, Center for Infectious Diseases, Heidelberg University — [3]School of Public Health and Malaria Research Institute, Johns Hopkins University

Plasmodium sporozoites, the slender forms of the malaria parasite injected by mosquitoes into the skins of their vertebrate hosts, provide a medically highly relevant model system for active chiral particles. Using 3D tracking in synthetic hydrogels, we show that sporozoites consistently move on right-handed helical trajectories. When they encounter a two-dimensional substrate, they switch to clockwise circular motion, whereas circling on glass in medium occurs with the opposite sense of rotation, suggesting on glass they try to invade the medium above. Using a sandwich assay, we demonstrate that chirality also determines the reverse transition from two-dimensional to three-dimensional motion. Combining these measurements with a theory for gliding motility allows us to identify the likely origin of chirality, namely an asymmetric distribution of adhesins. After confirming this via two-sided traction force microscopy, we finally use STED super-resolution microscopy to reveal a corresponding tilt in the apical ring complex. In summary, our analysis thus uncovers both the biological relevance and the molecular basis of chirality in the movement of malaria parasites.

CPP 1.5 Mon 10:30 BAR/SCHÖ

Squirmer dynamics in porous environments — •Mirko Residori[1], Christina Kurzthaler[1], and Sebastian Aland[2] — [1]Max Planck Institute for the Physics of Complex Systems — [2]TU Freiberg

We introduce a computational framework for simulating the dynamics of micro-swimmers in complex porous environments. Specifically, we adopt a diffusive domain approach to represent the surface of a micro-swimmer, modeled as a squirmer. This method ensures accurate and stable finite-element simulations, even in highly confined geometries. Validation against analytical and numerical benchmarks confirms the model*s accuracy and robustness. We then apply it to explore squirmer motion in heterogeneous porous media, revealing how hydrodynamic interactions lead to behaviors such as dynamic trapping due to hydrodynamically induced re-orientations. Moreover, we demonstrate that the squirmer parameter and the repulsive potential critically influence a squirmer's ability to navigate and escape confinement. The proposed framework offers a versatile and efficient tool for studying active motion in complex fluids and provides new insights into micro-swimmer transport and control in natural and engineered systems.

CPP 1.6 Mon 10:45 BAR/SCHÖ

Dynamics of passive tracers in active dumbbell suspension — •Chandranshu Tiwari and Sunil P. Singh — Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India.

The transport of passive tracers in active fluids exhibits rich dynamics arising from persistent interactions between active agents and the tracer. In our work, we employ Brownian dynamics simulations to investigate the dynamical behaviour of both isotropic(circular) and anisotropic(elliptical) tracers in active dumbbell suspension, considering only steric interactions. For circular tracers, we find that the speed shows a crossover from monotonically decreasing to increasing with tracer size as the dumbbells' speed is increased. The tracer's effective diffusion also displays a non-monotonic dependence on area fraction: the diffusivity first increases and then decreases at higher area fractions.

For anisotropic tracers, the characteristic non-monotonic trend persists. Moreover, their motion along the major and minor axes differs significantly. Anisotropic accumulation of active particles around the tracer generates direction-dependent forces and fluctuations, favouring motion along the major axis. Consequently, both the speed and diffusivity along the major axis exceed those along the minor axis.

15 min. break

Invited Talk CPP 1.7 Mon 11:15 BAR/SCHÖ

Modeling and inference of magnetotactic motility in complex environments — •Stefan Klumpp — Institute for the Dynamics of Complex Systems, University of Göttingen, Göttingen, Germany

Magnetotactic bacteria orient themselves and swim along field lines of the geomagnetic field. Their magnetically directed self-propelled motion makes them an instance of dipolar active matter. Here we focus on the interaction of these bacteria with walls or obstacles. Experiments in microfluidic systems show that interactions with walls result in (possibly transient) alignment parallel to the wall, which may compete with the alignment with the magnetic field. The dynamic behavior arising from the competition of the two alignments includes U-turn trajectories in circular chambers and trapping and escape dynamics in channels with overlapping cylindrical obstacles. In a phenomenological picture, the resulting motion can be described in an Active Brownian Particle model by introducing a wall torque that competes with the magnetic torque, which results in good agreement with experimental observations. Systematic Bayesian inference of the wall torque from observations shows that only a part of the torque function (dependence on incident angle) can be learned reliably from the data.

CPP 1.8 Mon 11:45 BAR/SCHÖ

Quantifying aggregation behaviour of filamentous cyanobacteria — •Elias Illing and Stefan Karpitschka — Fachbereich Physik, Universität Konstanz

Cyanobacteria are ubiquitous in nature, frequently causing ecological and economic harm by explosive growth, so called blooms.

We investigate the collective dynamics of entangled filamentous cyanobacteria in open liquid media, reminiscent of their aggregates found during later stages of blooms. We investigate the impact of illumination on the clustering and spreading of the bacteria and quantify the morphology of the bacterial aggregates by image analysis. We determine the critical density necessary for initial clustering and track the evolution of the subsequent stages, ranging from stable clusters to spreading mats. These states can be modulated by light intensity variations, potentially allowing for control of the morphological evolution of cyanobacterial aggregates.

CPP 1.9 Mon 12:00 BAR/SCHÖ

Dynamically Induced Spatial Segregation in Multi-Species Bacterial Bioconvection — •Mingqi Yan[1,2], Chenxi Wang[3], Oscar Gallardo-Navarro[4], Rinat Arbel-Goren[4], Joel Stavans[4], and Erwin Frey[1,2] — [1]Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, 80333 München, Germany — [2]Max Planck School Matter to Life, Hofgartenstraße 8, 80539, München, Germany — [3]School of Science, Harbin Institute of Technology, 518055, Shenzhen, China — [4]Department of Physics of Complex Systems, Weizmann Institute of Science, 7610001, Rehovot, Israel

Bacterial bioconvection is a classic example of collective behavior in active matter, where upward-swimming bacteria create density instabilities leading to large-scale fluid flows. While this phenomenon is well-studied in single-species suspensions, natural environments are typically inhabited by diverse microbial communities. Here, we investigate the collective dynamics of multi-species bacterial suspensions. Combining experiments with a continum model, we show that different bacterial species can spontaneously segregate into stable, spatially interlocked domains. Our theoretical analysis reveals that this segregation is not driven by biochemical antagonism but rather by the interplay between species-specific motility characteristics and the self-generated hydrodynamic flows. This work provides new insights into how physical interactions alone can drive the spatial organization of complex microbial communities.

CPP 1.10 Mon 12:15 BAR/SCHÖ

Light-switchable microbial rafts at air-liquid interfaces — •Gustav F. Nolte, Alexandros A. Fragkopoulos, Timo Völkl, Mechthild Rappold, and Oliver Bäumchen — University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany

In biological active matter, clustering occurs across a wide range of time and length scales, from molecular assemblies such as actomyosin networks to macroscopic systems like fire ant rafts. Here, we report on a fast, light-switchable, and fully reversible clustering phenotype on the microscale, observed at air-liquid interfaces: the raft formation of the biciliated microalga *Chlamydomonas noctigama*.

C. noctigama is a relative of the model organism *Chlamydomonas reinhardtii*, which exhibits light-switchable adhesion and subsequent clustering at solid-liquid interfaces [1,2]. We show how the cluster morphology depends on cell density and discuss potential growth mechanisms by analyzing dynamics of individual clusters. Furthermore, we characterize the dependence of raft formation on the light spectrum and interfacial free energy. Using micropipette force spectroscopy [3], we show that single cells exploit capillary forces for light-switchable ciliary adhesion to the air-liquid interface, enabling raft formation. In their natural habitats, reversible clustering may provide an advantage by allowing cells to accumulate in locations optimal for photosynthesis while increasing resilience to environmental stress.

[1] C. T. Kreis, et al., *Nat. Phys.* **14**, 45 (2018).
[2] S. Till, et al., *Phy. Rev. Res.* **4**, L042046 (2022).
[3] M. Backholm and O. Bäumchen, *Nat. Protoc.* **14**, 594-615 (2019).

CPP 1.11 Mon 12:30 BAR/SCHÖ

Circadian gravitaxis: Photosynthetic microswimmers remodel local pH to actively tune vertical migration — Arkajyoti Ghoshal[1], Soumitree Mishra[1], Jayabrata Dhar[2], Hans-Peter Grossart[3,4], and •Anupam Sengupta[1,5] — [1]Physics of Living Matter, Department of Physics and Materials Science, University of Luxembourg, Luxembourg — [2]Department of Mechanical Engineering, National Institute of Technology Durgapur, India — [3]Department of Plankton and Microbial Ecology, Leibniz Institute of Freshwater Ecology and Inland Fisheries, Stechlin, Germany — [4]Institute of Biochemistry and Biology, Potsdam University, Germany — [5]Institute for Advanced Studies, University of Luxembourg, Luxembourg

Motile phytoplankton shuttle between bright surface waters and deeper nutrient rich layers, usually controlled by internal circadian clocks. Yet many species show irregular movements, defying the expected circadian rhythm. Studying a bloom forming photosynthetic species, we found that cells adjust their vertical migration by altering local pH, mediated by a shift in their gravitactic behavior. This self-modulation of pH generates sub-populations which are physiologically similar but swim differently, remaining vertically separated even under uniform conditions. Supported by a cell-level analysis and mathematical model, we confirm that the pH-mediated circadian shift is underpinned by morphological adjustments. Our results support a circadian gravitactic model in which diurnal pH control drives diversified migration, enhancing fitness particularly in acidifying oceans.

CPP 2: Sustainability: Challenges and Solutions (joint session UP/CPP/SOE)

Accompanying session to Symposium SYSC

Time: Monday 9:30–10:30 Location: MER/0002

CPP 2.1 Mon 9:30 MER/0002

Making a university climate neutral: First experiences from implementing a Climate Protection Strategy at the University of Greifswald — •Christoph G. Hoffmann, Tiemo Timmermann, and Christian von Savigny — University of Greifswald, Greifswald, Germany

With a resolution of its Academic Senate, the University of Greifswald has in 2021 set the goal to achieve climate neutrality by the end of the decade.

While the aim of achieving climate neutrality within a few years is expectedly ambitious, a university as a bigger research institution has also a unique combination of knowledge to achieve it. This has already led to synergies from which particularly the teaching in the environmental subjects can benefit due to "home-made" practical experiences. This makes the whole University a living lab, in which the opportunities but also challenges of necessary transformations can be explored in an assessable setting.

Therefore, also the environmental physics group aims at contributing to and benefiting from this process. While our group is originally focused on basic atmospheric research, we cover a broader range of environmental physics topics in teaching, which overlap with the needs of the transformation process.

In this talk, we will give a short overview of the Climate Protection strategy of the University of Greifswald before we show some examples from our own work regarding the energy consumption of buildings.

CPP 2.2 Mon 9:45 MER/0002

Life Cycle Assessment practices for PV technologies: systematic literature review — •Zeena Patel — Technische Universität Ilmenau

In response to the growing importance of sustainability in solar energy development, this study addresses critical gaps in the application of Life Cycle Assessment (LCA) to photovoltaic (PV) technologies. A systematic review of 48 recent LCA studies across first-, second-, and third-generation PV systems was conducted to evaluate current practices, identify methodological inconsistencies, and highlight emerging trends. Despite increasing research interest and technological diversification, substantial variability exists in the definition of functional units, system boundaries, and impact categories, which hinders comparability and reproducibility. The widespread reliance on secondary databases and the limited use of primary, site-specific data further constrains the accuracy of environmental impact assessments. Additionally, the underutilization of Life Cycle Costing (LCC) and inconsistent application of sensitivity analyses reveal significant gaps in comprehensive sustainability evaluation. To advance the field, this study proposes standardization of LCA methodologies, improved data transparency, and expansion of impact categories beyond global warming potential to include toxicity and resource depletion. These measures are essential for enhancing the robustness, reliability, and policy relevance of PV LCA studies, thereby supporting sustainable innovation and deployment in the solar energy sector.

CPP 2.3 Mon 10:00 MER/0002

Electrochemical Modeling of SOFCs with Emphasis on Microkinetic and Anode Overpotential — •Iram Gul[1], Gabriela Soffiati[2], and Thiago Lopes[3] — [1]Research Center for Greenhouse Gas Innovation, University of São Paulo (USP), 05508-030, São Paulo * SP, Brazil — [2]Institute of Physics (IFUSP), University of São Paulo, Universidade, R. do Matão, 1371 - Butantã, São Paulo - SP, 05508-090 — [3]Research Center for Greenhouse Gas Innovation, University of São Paulo (USP), 05508-030, São Paulo * SP, Brazil

This study investigates Solid Oxide Fuel Cells (SOFCs) using a CO/H fuel mixture, focusing on thermodynamics, mass transport, and electrochemical kinetics. Thermodynamic properties such as heat capacity, enthalpy, entropy, and Gibbs free energy were analyzed across 600-800°C using MATLAB simulations. The Dusty Gas Model (DGM) revealed key mass transport behaviors in the anode, while Density Functional Theory (DFT) using VASP provided insights into surface reaction mechanisms. A microkinetic model examined the impact of anode overpotential on reaction kinetics and cell performance. Results show that higher temperatures improve mass transport and reduce Ohmic losses but slightly decrease the thermodynamic driving force. This multi-scale model enhances our understanding of SOFC behavior and offers a basis for improving fuel cell efficiency and material performance.

CPP 2.4 Mon 10:15 MER/0002

Thermal stability of ceria-zirconia oxides(CeZrO4) nanoparticles using combustion synthesis for the CO oxidation and NOx reduction — •Hamza Mohamed — IMMM, UMRS 6283 CNRS, Le Mans Université, Bd O. Messiaen, 72085 Le Mans Cedex 09, France

The study presents a green synthesis approach for fabricating ceria-zirconia oxide nanoparticles (CeZrO4 NPs) using the solution combustion synthesis method. The synthesized CeZrO4 nanoparticles were characterized using various sophisticated instruments and methods to determine their detailed properties. The UV-Vis spectra showed a characteristic absorbance peak at 242 nm and a band gap (Eg) of 3.05 eV. Simultaneously, Fourier transform infrared spectra of CeZrO4 NPs displayed bands at 418 cm-1, 991 cm-1, 1382 cm-1, 1658 cm-1, 2306 cm-1, 3288 cm-1, and 3643 cm-1, which indicates the presence of phytochemicals that facilitate the reduction and stabilization of CeZrO4 NPs. The major peaks for cubic CeZrO4 NPs were obtained with a crystalline size of 9.6 nm by X-ray diffraction. The microscopic analyses revealed irregular, ovoid, and aggregated morphologies with sizes ranging from 3 to 10 nm. The XPS analysis revealed the existence of Ce3d, Zr3d, C1s, and O1s states with their corresponding atomic percentages. Therefore, this investigation focuses on synthesizing catalysts that demonstrate both thermal stability and high catalytic activity for the oxidation of CO and the reduction of NOx.

CPP 3: French-German Session: Membranes and Porous Materials I

Time: Monday 9:30–11:00 Location: ZEU/LICH

Invited Talk CPP 3.1 Mon 9:30 ZEU/LICH

Theory and Modeling of Fluid Adsorption and Transport in Nanoporous Materials

— •Benoit Coasne — CNRS/University Grenoble Alpes, Grenoble, France — Institut Laue-Langevin, Grenoble, France

Nanoporous materials are at the heart of numerous important applications: adsorption (gas sensing, chromatography), energy (hydrogen storage, fuel cells and batteries), environment (phase separation, water treatment, nuclear waste storage), etc. Among these materials, nanoporous solids which have pores of the order of nm (e.g. active carbons, zeolites), are particularly interesting as ultraconfinement in their porosity leads to novel adsorption and transport phenomena. In this talk, we will present how molecular simulation and statistical physics allows developing models for adsorption and transport in these extremely confining materials. We will see how simple thermodynamic modeling allows rationalizing adsorption by considering reminiscent capillarity at vanishing lengthscales. Then, we will show how transport in nanoporous media can be described without having to rely on macroscopic concepts such as hydrodynamics. In particular, using parameters and coefficients available to experiments, we will see how transport coefficients can be rigorously upscaled using simple models such as intermittent brownian motion and free volume theory.

CPP 3.2 Mon 10:00 ZEU/LICH

Optimizing the Fabrication of Isoporous Block Copolymer Membranes by Concurrent Multi-fidelity Simulations

— •Gregor Häfner and Marcus Müller — Institute for Theoretical Physics, University of Göttingen, Germany

Integral-asymmetric copolymer membranes promising promising class of functional macromolecular systems with diverse potential applications, including water purification and protein separation. Their fabrication is a two-step process: solvent evaporation and subsequent nonsolvent-solvent exchange to create an isoporous top-layer, and a spongelike substructure. We model the process using two complementary schemes – a highly coarse-grained, particle-based model that treats the polymer chains directly, and a continuum model, describing the system only by its concentration fields. To exploit the accuracy of the former while retaining the efficiency of the latter, we couple these for a concurrent multi-fidelity simulation. The continuum simulation treats the whole system, spawning a particle-based simulation in the region of its lowest accuracy. For this, a neural network is employed to estimate the future error and guide the decision of the subdomain position. We achieve a tenfold increase in computational efficiency compared to pure particle-based simulations, enabling us to investigate large film depths. Our simulations delineate a process window for successful membrane fabrication, which fully match the experimentally accessible parameters, showing an isoporous top layer, a porous substructure and finger-like macrovoids, allowing us to guide experimental membrane optimization.

CPP 3.3 Mon 10:15 ZEU/LICH

In situ monitoring of relaxation dynamics in polyethylenimine during CO2 absorption and desorption

— •Martin Tress — Peter Debye Institute for Soft Matter, Leipzig University

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) [1]. Upon CO2 absorption, thin film PEI shows a slower dynamics, which is consistent with an elevated glass transition temperature revealed in complementary differential scanning calorimetry measurements. Insitu kinetics measurements in thin film samples as well as PEI-infused porous silica demonstrate complex changes in the overall permittivity as well as relaxation times and relaxation amplitudes of some processes during CO2 sorption or desorption. This suggest an intriguing interplay between physical and chemical CO2-sorption, diffusion and the dynamics of PEI. Finally, a tentative model will be presented to describe the observed curves qualitatively. These results demonstrate that BDS is a powerful in-situ-platform to resolve the temporal dynamical changes of polyamines and their impact on sorption kinetics, and may inform specific system adjustments to improve CO2 capture performance.

[1] M. Tress, S. Ahmadi and S. Cheng, AIChE J. 71 (2025) e18627

CPP 3.4 Mon 10:30 ZEU/LICH

Scalable and Tunable Carbon Nanomembranes for Selective Molecular Transport

— •Zhen Yao[1], Jan Biedinger[1], Martin Wortmann[1], Nikolaus Meyerbröker[2], Yang Yang[1], Andreas Hütten[1], Günter Reiss[1], and Armin Gölzhäuser[1] — [1]Bielefeld University, Bielefeld, Germany — [2]bCNM Technologies GmbH, Bielefeld, Germany

Carbon nanomembranes (CNMs), molecularly thin two-dimensional materials with intrinsic sub-nanometer pores, provide a versatile platform for nanofluidics. Their ultrathin structure enables fast molecular flux, while surface chemistry and pore architecture can be tailored for selective transport. We present a scalable synthesis route based on electron-induced crosslinking of spin-coated poly(4-vinylbiphenyl) films, combined with atomic layer deposition (ALD) for pore and surface functionalization. This strategy enables precise tuning of pore dimensions and hydrophilicity, yielding CNMs with water vapor permeance as high as 1.9×10^{-5} mol s^{-1} m^{-2} Pa^{-1} and H_2O/N_2 selectivity above 10000, outperforming state-of-the-art polymer and graphene oxide membranes. These results establish CNMs as promising candidates for energy-efficient dehumidification and gas separation. Together, these studies demonstrate how scalable fabrication and nanoscale interface engineering translate into tunable nanofluidic transport, highlighting CNMs as a versatile materials platform for separations, sensing, and controlled molecular flow.

CPP 3.5 Mon 10:45 ZEU/LICH

Is it possible to use nano-confined water for cloaking or magnifying of static electric fields?

— •Kira Fischer[1], Julia Brandt[1], Philipp Stärk[2], Alexander Petrov[1], and Alexander Schlaich[1] — [1]Hamburg University of Technology — [2]University of Stuttgart

Assuming radial anisotropy in the dielectric response of water in cylindrical or spherical confinement, Kettunen et al., have shown that for certain ratios of permittivity contrast it is possible to cloak the interior sample, or to magnify the response of an inner cylinder. Indeed, water at interfaces and in confinement shows a strongly anisotropic dielectric response, with high dielectric permittivity in parallel and low permittivity perpendicular to the interface, as observed experimentally by Fumagalli et al.

Here, we probe the radial and azimuthal dielectric response of water in cylindrical confinement. We do so by calculating the dielectric permittivity profile from molecular dynamics simulations, both using a Green-Kubo relation as well as applied fields. Near the interface, we observe a high dielectric permittivity in the azimuthal direction and a low dielectric permittivity in the radial direction of the cylinder, supporting the concept of radial anisotropy.

Applying a static, homogenous external field we then analyse the resulting water polarization. The observed effective response of water inside a cylinder is almost bulk like, and no significant cloaking effect is observed. We use effective medium theory to rationalize this behavior and discuss possible applications of cloaking in model fluids.

CPP 4: Energy Storage Materials and Devices I

Time: Monday 9:30–11:15 Location: ZEU/0255

Invited Talk CPP 4.1 Mon 9:30 ZEU/0255

Exploration of Cathode Materials for Li-S Batteries — •Yan Lu — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Recently, a lot of efforts have been devoted into lithium-sulfur (Li-S) battery system due to its high theoretical capacity (1675 mAh g-1) and low cost, which could be a competitive candidate for the next-generation batteries in the future. However, it suffers from a poor cycling stability during charging-discharging, which is blamed to the "shuttle effects" of lithium polysulfides. Fundamental understanding of the formation and dissolution processes of both solid phases, S8 and Li2S, is necessary for the development of advanced cathode materials (both organosulfur and metal compound-based sulfur host) with improved electrochemical performance. Synchrotron-based operando high-resolution X-ray imaging has been successfully used for the detailed morphology study of sulfur particles during cycling of the battery cells. Using colloidal route, complex hybrid carbon nanostructures have been synthesized using colloidal polymeric particle as soft template, which have been applied as cathode materials for Li-S batteries.

CPP 4.2 Mon 10:00 ZEU/0255

Temperature-dependent Crystal Structure of Dimethyl Carbonate — •Lea Westphal[1,2], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]MLZ, TUM, Garching, Germany

The performance and safety/stability of Li-ion batteries (LIBs) can be enhanced by optimizing the charge-storing electrode materials and/or the charge-mediating liquid electrolytes. In LIB research, the major focus has been on the electrode subsystem, while liquid electrolytes are studied much less. Upon cooling of LIBs to investigate their performance at low temperatures, a series of Bragg reflections has been observed, which was assigned to the freezing of liquid electrolyte. Further measurements reveal the development of long-range order in the model electrolyte mixture LP30. To better understand this emerging order, it is essential to investigate the system's individual components, especially under conditions near room temperature relevant to in situ sub-ambient LIB studies.

This contribution outlines our efforts to crystallize Dimethyl Carbonate with minimized preferred orientation, in order to study the unit cell across the entire solid temperature range using neutron- and synchrotron-based powder diffraction. The datasets are complemented by synchrotron single-crystal diffraction experiments. Additionally, the liquid state is investigated by Total Scattering and Pair Distribution Function analysis.

CPP 4.3 Mon 10:15 ZEU/0255

Electron Energy Loss Spectroscopy for oxidation state analysis on ammonia synthesis catalysts — •Daniela Ramermann, Michael Poschmann, Elisabeth H. Wolf, Holger Ruland, and Walid Hetaba — Max-Planck-Institut für Chemische Energiekonversion, Mülheim (Ruhr)

Electron energy loss spectroscopy (EELS) is a powerful technique, not only for the determination of elemental compositions, but also for the investigation of chemical bonding and oxidation states. For the analysis of EELS data, the use of cross-section models is quite common, but the use of reference spectra improves the quantification results. In addition, it allows for the fitting of the edge shapes to investigate oxidation states with the spatial resolution of the electron microscope.

Because the available databases for EELS references [1] are not exhaustive, reference materials are obtained from acquired commercial materials of well-known and defined properties. It is crucial to thoroughly characterize these materials before measuring the reference spectra, as the materials may have local impurities or differ from the desired oxidation state. For the Fe-based catalyst system some reference materials are of mixed oxidation state, presenting an additional challenge.

We show the process of acquiring suitable EELS references for materials used in catalysis and the application of mapping the oxidation state and phase composition on a Fe based ammonia synthesis catalyst.

[1] https://eelsdb.eu, https://eels.info/atlas

CPP 4.4 Mon 10:30 ZEU/0255

Investigating the Conversion Reaction of the Cathode Active Material FeS$_2$ in Solid-State Batteries via Transmission Electron Microscopy — •Franziska Hüppe[1], Matilde Pavan[2], Shamail Ahmed[1], Jürgen Belz[1], Jürgen Janek[2], and Kerstin Volz[1] — [1]Philipps-Universität Marburg, Department of Physics and mar.quest, Hans-Meerwein-Straße, 35043, Marburg, Germany — [2]Justus-Liebig-Universität Gießen, Institute of Physical Chemistry and Center for Materials Research, Heinrich-Buff-Ring, 35392, Gießen, Germany

Solid-state batteries are particularly promising for high-energy storage, as they potentially allow for the use of electrode materials with higher specific capacities. In the case of FeS$_2$ as cathode active material, also the cost effectiveness and the environmental impact would be drastically enhanced. However, FeS$_2$ is a conversion-type material that undergoes continuous compositional and structural changes during cycling that is not yet fully understood at the micro- and nanoscale.

Scanning transmission electron microscopy (STEM) offers structural insights at high resolution and is combinable with deepening investigation methods like energy dispersive X-ray spectroscopy (EDX) and electron energy loss spectroscopy (EELS) to identify the different compounds forming during different depth of discharge (lithiation).

The pristine, uncycled cathode sheet contains FeS$_2$ particles with cubic structure. With increasing depth of discharge, the particles react from the outside in, forming core-shell structures. The multimodal STEM analysis will be discussed in detail during the presentation.

CPP 4.5 Mon 10:45 ZEU/0255

Dual-cation pre-intercalated hydrated vanadium oxide for ultralong cycling stability in aqueous zinc-ion batteries — •Yan Ran, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

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 4.6 Mon 11:00 ZEU/0255

Unveiling the Interfacial Behavior of Lithium Batteries by Operando X-ray Scattering — •Yuxin Liang[1], Fabian Apfelbeck[1], Kun Sun[1], Yingying Yan[1], Lyuyang Cheng[1], Guangjiu Pan[1], Tianle Zheng[1], Yajun Cheng[2], Anton Davydok[3], Christina Krywka[3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]College of Renewable Energy, Hohai University, Changzhou, China — [3]Helmholtz-Zentrum Hereon, Geesthacht, Germany

Poly(ethylene oxide) based solid composite electrolytes suffer from poor conductivity and lithium dendrite growth, especially toward the metallic lithium metal anode. In our recent work, we focus on the fabrication and comprehensive characterization of performance-enhanced PEO-based composite electrolytes for lithium batteries. Advanced nano-focus X-ray scattering techniques were used to investigate the interfacial behavior within the lithium metal battery, as well as its failure mechanisms. With the modification of plasticizer, the electrolyte exhibit good electrochemical performance and interfacial compatibility. However, the reference electrolyte exhibit early dendrite formation from the lithium surface into the electrolyte, leading to persistent structures that degrade performance. The results highlight the potential of these fabrication and analysis methods, demonstrating their application in advancing lithium battery technologies and contributing to the development of cutting-edge characterization techniques.

CPP 5: Wetting, Fluidics and Liquids at Interfaces and Surfaces I (joint session CPP/DY)

Time: Monday 9:30–11:00 Location: ZEU/0260

Invited Talk CPP 5.1 Mon 9:30 ZEU/0260

Cleaning of dusty surfaces — •Doris Vollmer[1], Franziska Sabath[1], Abhinav Naga[2], Stefanie Kirschner[1], Tarik Karakaya[1], Rüdiger Berger[1], Hans-Jürgen Butt[1], and Halim Kusumaatmaja[2] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]Ackermannweg 10

The accumulation of dust, sand or other contaminants on solar modules leads to significant efficiency losses. Billions of litres of water are used annually to clean solar modules, and other natural or manmade surfaces. However, the complex interplay between capillary and frictional forces, which determines successful removal or unwanted redeposition, is still poorly understood. By combining confocal microscopy and Boltzmann lattice simulations, we observe and quantify the removal of particles from smooth and rough surfaces by a water droplet, varying the hydrophobicity of the surface and the particles. Hydrophilic particles aquaplane, resulting in negligible friction and easy particle removal. For hydrophobic particles, the tangential component of the capillary force promotes or counteracts particle removal. Undesirable redeposition depends on the number and wettability of the particles. On superhydrophobic surfaces, the small contact area facilitates easy removal. For individual particles, we propose a phase diagram for particle removal.

CPP 5.2 Mon 10:00 ZEU/0260

Marangoni contracted droplets on Textured Surfaces: Insights from Lubrication Theory — •Raphael Saiseau, Ze Xu, and Stefan Karpitschka — Fachbereich Physik, Universität Konstanz, 78464 Konstanz, Germany

Wetting and evaporation of droplets on micropatterned surfaces are central to both natural processes and technological applications, from anti-icing and spray cooling to inkjet printing and semiconductor processing. Droplet behavior on such surfaces is set by surface chemistry and topography, and most control strategies traditionally rely on specific materials or designs, limiting their versatility.

By depositing droplets on top of a pillars-decorated substrate in a vapor-controlled chamber, we show that the spreading and wicking can be controlled, and even temporarily suppressed, by using the vapor of a second, low-surface tension liquid, generating Marangoni stresses through its condensation near the droplet edge. We present numerical and semi-analytical solutions of the thin film equation coupled to a composition evolution equation, and diffusion-limited evaporation. The wicking effect of the texture is implemented through an effective height-dependent pressure, analogous to classical hemiwicking models. The emerging Marangoni flows oppose the prevailing capillary flows, leading to a quasi-stationary rather than a spreading or wicking drop. We derive a predictive relation between material parameters and drop shape, opening the way for designing controlled coating, cleaning and drying strategies on textured surfaces.

CPP 5.3 Mon 10:15 ZEU/0260

Photoswitchable Arylazopyrazole Monolayers on Aluminum Oxide for Tunable Wettability — •Tim Blinzer, Christian Honnigfort, and Björn Braunschweig — Institute of Physical Chemistry and Center of Soft Nanoscience, University of Münster, Corrensstraße 28-30, Münster 48149, Germany

Smart surfaces that can change their wettability on demand are interesting for applications such as self-cleaning or microreactors. To tune the surface wettability, we functionalized aluminum oxide surfaces with arylazopyrazole (AAP) phosphonic acids using a Langmuir-Blodgett transfer. AAP molecules in the deposited monolayers undergo reversible E/Z photoisomerization driving changes in surface wettability. This was investigated as a function of surface coverage, where the responsiveness—i.e. the changes in molecular structure and in the apparent contact angle—was studied in detail. Here time-dependent sum-frequency generation (SFG) was used to obtain in situ information on the dynamic changes in monolayer upon E/Z switching with 520 nm green and 365 nm UV light. Furthermore, we show that increasing surface roughness by depositing nanoaggregates of the AAP phosphonic acid leads to a drastic increase in the change of the contact angle when switching from the E to the Z isomer. Indeed, the change in contact angle increased from only 7° for homogeneous monolayers to about 20° for nanostructured surfaces using AAP aggregates.

CPP 5.4 Mon 10:30 ZEU/0260

Motion and interaction of Marangoni contracted droplets on micropatterned surfaces — •Ze Xu, Raphael Saiseau, and Stefan Karpitschka — Fachbereich Physik, Universität Konstanz, Konstanz, Germany

Wetting of micropatterned surfaces is ubiquitous in nature and key to many technological applications like inkjet printing and semiconductor processing. Overcoming the intrinsic, chemistry- and topography-governed wetting behaviors often requires specific materials, leading to contradicting requirements between the processing strategy and the final product. Here, we demonstrate that droplet spreading and wicking on hydrophilic patterns can be controlled by the vapor of a lower-surface-tension liquid. Condensation of the vapor induces Marangoni forces that delay capillary wicking and contract liquid into a droplet on top of the imbibed film. Consequently, a Marangoni-contracted droplet coexists with a finite imbibition film for prolonged times. We demonstrate how these droplets interact with each other, both by their vapor cloud, and by the imbibed liquid film that surrounds them. Modulating the ambient vapor, also these interactions can be modulated, devising new strategies for coating, cleaning, and drying functional surfaces.

CPP 5.5 Mon 10:45 ZEU/0260

Wetting of Swelling Polyelectrolyte Surfaces on a Macroscopic and Nanoscopic Scale — •Mona Meltschoch and Regine von Klitzing — Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

Wetting on adaptive polymer interfaces plays an important role in soft matter physics, particularly when spreading is affected by substrate hydration. Polyelectrolyte multilayers (PEMs) are suitable model systems because they absorb water and evolve across multiple time scales, creating a link between nanoscale polymer mobility and macroscopic contact line motion. PEM films were prepared by the layer-by-layer method, and their wetting behaviour was examined at different scales. Nanoscale morphology and hydration were characterised by atomic force microscopy (AFM), while macroscopic wetting was followed via optical contact angle (CA) measurements. Previous studies report a decrease in water CA on PSS-terminated PEMs under humid atmosphere. To assess how film architecture affects wetting, PEMs with varying bilayer numbers and terminal charge (PSS vs. PAH) were fabricated, showing smooth surfaces and a linear thickness increase. Current work explores AFM beyond static surface imaging by applying it directly to droplets on PEM films. This approach aims to track local swelling, interface deformation and contact line behaviour under liquid exposure. Measurements with different droplet liquids are being established, with the long-term goal to link nanoscale hydration dynamics to macroscopic changes in contact angle and wetting evolution.

CPP 6: French-German Session: Membranes and Porous Materials II

Time: Monday 11:15–12:45 Location: ZEU/LICH

Invited Talk CPP 6.1 Mon 11:15 ZEU/LICH

Hierarchical Porosity Meets Nanoconfined Water: Toward Water-Driven Functional Materials — •Patrick Huber — Hamburg University of Technology — Deutsches Elektronen-Synchrotron DESY

Natural materials achieve remarkable functionality using only simple chemical building blocks, relying on architectures that span multiple length scales. A key feature of many biological systems is their hierarchical porosity, which guides fluid transport from large channels down to nanopores where water acts as a nanoscale working fluid. In such confined spaces, water displays distinct structural dynamics and interfacial behaviour that strongly influence mechanical, transport, and optical responses. This contribution introduces a new class of sustainable water-driven materials whose active behaviour originates from the interplay between hierarchically porous solid networks and interfacial or nanoconfined water. These Blue Materials exploit water-mediated processes such as humidity-responsive actuation, capillary-driven transport, and pore-structure controlled optical effects. Their functionality is rooted in the precise design of their pore architecture, especially at the nanoscale where confined water governs dynamic material behaviour. Beyond emulating natural processes, these principles open pathways for harvesting electrical energy from environmental wetting-drying cycles, offering a sustainable approach to energy generation in porous materials.

CPP 6.2 Mon 11:45 ZEU/LICH

Accessing topological properties of mesoporous materials via SDGW model — •Georgiy Baroncha[1], Rustem Valiullin[1], and Eustathios Kikkinides[2] — [1]Felix Bloch Insitute for Solid State Physics, Leipzig University, Leipzig, Germany — [2]Department of Chemical Engineering, Aristotle University of Thessaloniki, Thessaloniki, Greece

Gas sorption is commonly used to characterize mesoporous materials, but its ability to reveal how pores are interconnected remains limited due to an incomplete understanding of network effects on phase behavior. In this work, we represent mesoporous structures using statistically disordered Bethe, and apply a statistical-thermodynamic approach to interpret adsorption/desorption or melting/freezing phase transitions. We demonstrate that gas sorption analysis can be used not only to determine pore size distributions, but also to quantitatively infer the average interpore connectivity and correlations between pore diameters in the material. At the same time, we find that sorption isotherms are largely unaffected by other aspects of pore network topology. These results identify the key structural factors shaping sorption behavior and broaden the capabilities of gas sorption for simultaneous assessment of pore size distribution and mean connectivity in mesoporous materials.

CPP 6.3 Mon 12:00 ZEU/LICH

2D Water in Clay Nanoconfinement: Tiny Space for Large Implications — •Vasily Artemov — Hamburg University of Technology

This talk presents recent advances in understanding the behavior of two-dimensional water in clay nanoconfinement, with a focus on its dielectric properties. Although clays are abundant, their crystal particles typically lack directional alignment. I will discuss an approach for self-assembling clay particles into large, scalable membranes in which the flakes are oriented parallel to each other, enabling a controlled and reproducible platform for studies of confined water at the nanoscale. Using this self-assembled nanofluidic platform, I will present experimental evidence of confinement-induced charge-separation effects that support electricity storage in water channels of 1 nm wide [1]. By combining insights from nanoscale physics, electrochemistry, and materials science, I will highlight how confinement within clay interlayers can influence ion transport, energy-storage phenomena, and our broader understanding of water at the interfaces.

[1] V. Artemov, S. Babiy, Y. Teng, J. Ma, A. Ryzhov, T.-H. Chen, L. Navratilova, V. Boureau, P. Schouwink, M. Liseanskaia, P. Huber, F. Brushett, L. Laloui, G. Tagliabue, A. Radenovic, Bulk electricity storage in 1-nm water channels, arXiv:2410.11983 (2024)

CPP 6.4 Mon 12:15 ZEU/LICH

Two coexisting populations of sorbed DMSO drive distinct structural changes in a swelling porous material — Raimund Teubler[1,3], Alexandra Serebrennikova[1,2,3], Maximilian Fuchs[1,3], Eduardo Machado Charry[1], Robert Saf[1], Erich Leitner[1,3], and •Karin Zojer[1,3] — [1]Graz University of Technology, Graz, Austria — [2]Wood Kplus Competence Center, Linz, Austria — [3]CDL for mass transport through paper, Graz, Austria

Understanding the swelling of cellulose-lignin-based fibers is essential for describing the mechanisms governing water and volatile uptake in porous materials such as paper. We reveal the dynamics of dimethyl sulfoxide (DMSO) uptake and quantify the resulting changes in fiber and sheet structure by combining three recently developed techniques based on concentration determination in coupled uptake/release experiments, microcomputed tomography (μ-CT), and optical microscopy. DMSO interacts with the fibers in a manner similar to water. We show that DMSO is incorporated into the paper sheet in two distinct populations, each contributing differently to the structural evolution of the material. The first population consists of DMSO molecules incorporated into the fibers, leading to fiber swelling. The second population accumulates at the fiber surfaces; although these molecules bind to and are released from the surface rapidly, they gradually modify the fiber surface [1]. As a consequence, built-in stresses within the fiber network are released, causing structural changes that persist long after fiber swelling has ceased.

[1] R. Teubler et al., DOI: 10.1007/s10450-025-00656-x.

CPP 6.5 Mon 12:30 ZEU/LICH

Electrochemical control of photoluminescence emission by a porous silicon membrane — •Manuel Brinker[1] and Patrick Huber[1,2] — [1]Institute for Materials and X-ray Physics, Hamburg University of Technology, Denickestr. 15, Hamburg 21073, Germany — [2]Centre for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, Hamburg 22607, Germany

Porous silicon is a highly versatile porous material with a broad range of exceptional properties. Due to the geometrical confinement of the pore walls, the band structure is strongly altered and the pore walls effectively act as quantum wires. Thus, photons are emitted in the visible range when the membrane is excited by a UV source. This optical effect has been widely researched and is the foundation for porous silicon to be applied, e.g., as a sensor material in the life sciences. Here, we study the influence of electrochemo-mechanical coupling on the photoluminescence performance. Thereby, charge carriers are accumulated in the electric double layer of a porous silicon electrode by charging it in an electrolyte solution. A change in surface stress at the interface with the porous material is induced and results in an overall mechanical reaction of the porous material. The strain acting on the pore walls consecutively influences the emission characteristics of the photoluminescence emission. An extensive in-situ study ascertains a highly linear dependence of the emission peak's wavelength on the charging state of the electrode. This research establishes the groundwork for porous silicon electrodes to be utilized as mechano-optical sensors.

CPP 7: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods I

Time: Monday 11:30–12:45 Location: ZEU/0255

CPP 7.1 Mon 11:30 ZEU/0255

Exploration of quantum-mechanical space towards olfactorial receptor and body odor volatilomes interaction — •Li Chen[1], Leonardo Medrano Sandonas[1], Shirong Huang[1], and Gianaurelio Cunibert[1,2] — [1]Institute for Materials Science and Max Bergmann Center for Biomaterials, TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TUD Dresden University of Technology, 010628 Dresden, Germany

We present the MORE-QX dataset generated from quantum-mechanical (QM) simulations of atomistic systems spanning diverse design stages for gas sensing. The dataset contains 23,838 and 10,441 BOV*receptor dimer systems in the gas phase and on graphene surfaces, respectively, to obtain sensing-related binding features. By analyzing the property space spanned by MORE-QX, we observe substantial flexibility in identifying interaction configurations with desired electronic binding characteristics, owing to the weak correlations among the properties. To gain insights into the complex interplay between these sensing properties, we construct tree-based machine-learning models for fast evaluation of binding features using only QM molecular properties, and combine them with an explainability framework to identify the key design factors of BOV*receptor systems that govern sensing performance. Our work provides valuable insights into the sensing mechanism and design principles of olfactorial receptors for BOV sensing.

CPP 7.2 Mon 11:45 ZEU/0255

Non-local diffusion model as a description for non-Gaussian diffusion in scattering experiments — •Harish Srinivasan[1,2], Veerendra Kumar Sharma[2], and Subhankur Mitra[2] — [1]Institute of Applied Physics, University of Tübingen, Tübingen, Germany — [2]Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, India

We introduce a non-local diffusion (NLD) model that provides a unified theoretical framework for describing non-Gaussian diffusive dynamics in fluids. The NLD formulation generalizes conventional diffusion by incorporating a jump kernel, enabling analytical characterization of van-Hove self-correlation functions with exponential tails. This framework naturally connects two major classes of anomalous transport observed in scattering experiments: non-Gaussian fractional Brownian motion (nGfBm) in sub-diffusive glass-formers, and Fickian yet non-Gaussian diffusion (FnGD) in cage-jump dominated liquids. In the nGfBm regime, the NLD description captures the crossover from non-Gaussian to Gaussian sub-diffusion seen in molecular and polymeric glass-formers [1]. In the FnGD regime, the NLD model predicts the exponentially fast approach to Fickianity and the much slower algebraic restoration of Gaussianity [2]. Comparison with incoherent quasielastic neutron scattering data across multiple systems demonstrates the universal applicability of the NLD model and establishes non-local diffusion as the common physical origin of non-Gaussian signatures in molecular fluids. [1] H. Srinivasan et. al., Phys. Rev. Lett. 132, 058202 (2024) [2] H. Srinivasan et. al., arXiv:2504.15020 (2025)

CPP 7.3 Mon 12:00 ZEU/0255

Optimizing EquiDTB potentials for large-scale molecular simulations — •Zekiye Erarslan, Gianaurelio Cuniberti, and Leonardo Medrano Sandonas — Chair of Materials Science and Nanotechnology, TUD Dresden University of Technology, 01062 Dresden, Germany

Density Functional Tight-Binding (DFTB) is a semi-empirical method that enables efficient large-scale simulations at moderate computational cost compared to first-principles quantum-mechanical methods. However, its generalizability is limited by the use of parameterized pairwise repulsive potentials. The recently developed EquiDTB framework [chemRxiv, 10.26434/chemrxiv-2025-z3mhh] has shown that replacing this repulsive term with a many-body ΔTB potential—trained using equivariant neural networks—significantly improves both the accuracy and transferability of the DFTB method. As a result, EquiDTB achieves hybrid DFT-PBE0 level accuracy across diverse electronic, structural, and vibrational properties of large molecules and molecular dimers containing C, N, O, and H atoms. In this work, we extend the EquiDTB framework by training a more general ΔTB potential on the chemical space covered by the newly generated QCML dataset. This expansion broadens EquiDTB beyond its original four-element scope and enables accurate simulations of neutral molecular systems containing C, N, O, H, P, S, Na, and Cl. We validate the performance of the optimized EquiDTB model through extensive calculations on large molecular dimers, RNA systems, and organic periodic materials.

CPP 7.4 Mon 12:15 ZEU/0255

MolecuTas: an ML platform for refining quantum properties and bioactivity of complex molecules — •Álvaro Vallejo Bay[1], Jannis Krüger[2], Thomas Hellweg[2], Gerardo Prieto[1], and Vicente Domínguez Arca[2,3] — [1]Applied Physics, University of Santiago de Compostela, Spain — [2]Physical and Biophysical Chemistry, Bielefeld University, Germany — [3]Biosystems and Bioprocesses Engineering, IIM-CSIC, Spain

This work introduces MolecuTas, a neural architecture designed for the ultrafast prediction of atomistic and molecular properties with accuracy approaching density functional theory, yet at negligible computational cost. The project tackles core challenges in computational chemistry, particularly the size dependence of predictive models and the loss of structural detail in conventional representations. To overcome these limitations, we develop a custom data extraction and molecular fragmentation pipeline based on large quantum datasets, ensuring the preservation of essential information such as connectivity, symmetries, chemical environments, and electronic features.

Building on this foundation, we propose a family of advanced Graph Neural Networks that explicitly integrate physicochemical principles and disentangle local from global information, enabling robust generalization across diverse molecular systems. Ultimately, MolecuTas aims to provide a reliable tool for molecular dynamics, enabling precise and fast prediction of partial charges and other key descriptors required for accurate simulations and next-generation chemical design.

CPP 7.5 Mon 12:30 ZEU/0255

Property-guided diffusion modeling for efficient exploration of chemical spaces — •Leonardo Medrano Sandonas[1], Michael Hanna[1], Julian Cremer[2], and Gianaurelio Cuniberti[1] — [1]TUD Dresden University of Technology, Germany. — [2]Pfizer Worldwide R&D, Germany.

The rational in silico design of chemical compounds requires a deep understanding of both structure-property and property-property relationships across chemical compound space, as well as efficient methodologies for defining inverse property-to-structure mappings. In this presentation, I will discuss our recent efforts to leverage the ”freedom of design” concept [Chem. Sci. 14, 10702 (2023)] in the chemical space of drug-like molecules to develop an efficient generative AI framework capable of designing molecular compounds with targeted quantum-mechanical (QM) properties. To this end, we have implemented a property-guided active learning approach that optimizes the performance of equivariant diffusion models within each property space. Generated molecules and their associated QM properties are validated through exhaustive DFT calculations at the PBE0+MBD level using the FHI-aims code. Our findings reveal a consistent improvement in property accuracy when guiding the diffusion model to explore less populated regions of the target property space. This performance is further enhanced by incorporating molecular building blocks into the initial training set. We expect our work to advance the development of sustainable generative AI frameworks for identifying molecules tailored to specific chemical processes.

CPP 8: Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)

Time: Monday 11:30–12:45 Location: ZEU/0260

CPP 8.1 Mon 11:30 ZEU/0260

Do the particle number and wettability affect their removability by a single water drop? — •Franziska Sabath[1], Abhinav Naga[2], Halim Kusumaatmaja[2], and Doris Vollmer[1] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]Institute for Multiscale Thermofluids, School of Engineering, University of Edinburgh, United Kingdom

The accumulation of dust on surfaces, *e.g.* windows and solar panels, is a well-known phenomenon in everyday life. The ratio of the capillary force between particles and drop and the resistive forces between particles and surface, *i.e.* friction and adhesion, determine whether the particles can be removed by a water drop. The likeliness of particle removal depends on both particle and surface wettability. It is still questionable how the particle arrangement, the total resistive force acting and the unwanted redeposition of particles depend on the number and wettability of the particles. Here, we investigate the removal of hydrophobic and hydrophilic spherical particles from a flat surface. As the number of hydrophobic particles increases, the total resistive force increases, but not linearly, and overcomes the capillary force, causing particle redeposition. In contrast, the hydrophilic particles slide on a thin water film, reducing the particle-surface friction and no resistive force is measured within our experimental resolution.

CPP 8.2 Mon 11:45 ZEU/0260

Modelling and simulation of capillary adhesion between rough surfaces — •Yizhen Wang, Martin Ladecký, and Lars Pastewka — University of Freiburg, Freiburg, Germany

At a small enough length scale, surfaces are always rough, regardless whether they are generated by nature or via artificial process. When two such surfaces are placed close enough, the water molecules in the humid air are adsorbed and hence form capillary bridges. Theories for adhesive interactions typically use simple cohesive laws, which are good models for Van-der-Waals interactions but may not be appropriate for capillary adhesion. We here construct a phase-field model that explicitly represents water present between two contacting rough interfaces. We show results obtained with this model on synthetic, computer-generated, self-affine rough interfaces. In quasi-static simulation, we observe the merging and splitting of droplets under the normal and shear movement of the interfaces. The overall force is dominated by the perimeter of the droplet, indicating the importance of a detailed understanding of droplet morphology.

CPP 8.3 Mon 12:00 ZEU/0260

Impact of surface wettability on the removal of montmorillonite aggregates by water drops How natural dirt is removed from various surfaces — •Stefanie Kirschner, Franziska. Sabath, Azadeh Sharifi-Aghili, Tarik Karakaya, and Doris Vollmer — Max Planck Institute for Polymer Research, 55128 Mainz, Germany

Natural dust on photovoltaic modules or windows, is a critical factor that reduces their performance. Previous experiments focused on the removal on single or many spherical particles. The removal of aggregates of natural particles, is not yet understood. Here, we focus on minerals, commonly present in desert dust. Using confocal laser scanning microscopy the detachment behavior upon contact with a water drop is measured on surfaces with different wettability. In addition, the force required to remove the aggregate by a sliding water drop was investigated. During drying on a hydrophilic surface, the dispersed particles cover a larger area. This increases the total contact area, resulting in higher adhesion and reduced detachment. In contrast, hydrophobic surfaces promoted more compact aggregates with improved removability. Finally, I will compare the detachment forces and the removal behavior of different natural aggregates, e.g. soot, salt and humic acid.

CPP 8.4 Mon 12:15 ZEU/0260

Equilibrium droplets on deformable substrates exhibit cloaking and demixing at the three-phase contact line — •Khalil Remini[1], Ralf Seemann[1], Dirk Peschka[2], and Barbara Wagner[2] — [1]Universität des Saarlandes — [2]Weierstrass Institute for Applied Analysis and Stochastics

This work examines the equilibrium shape of liquid droplets on viscoelastic PDMS substrates with varying elasticities. By combining atomic force microscopy (AFM) with an initial lift-off step, we reveal not only the top contour of the droplets but also the buried droplet*substrate interface. A second lift-off step provides additional structural details near the three-phase contact line (TPCL), where the interfacial tensions adopt a Neumann balance. Quantitative analysis of the reconstructed 3D droplet shapes shows that non-crosslinked, liquid PDMS molecules are extracted from the elastic network under stress and accumulate as a liquid rim around the droplet base, thereby altering both the droplet shape and the substrate profile close to the TPCL. These liquid molecules also cloak the droplets with a thin film, modifying the effective surface tensions. Furthermore, dewetting experiments demonstrate that this demixed liquid already appears at an early stage of dewetting and remains at an approximately constant amount throughout the process.

CPP 8.5 Mon 12:30 ZEU/0260

Tuning Sliding Drop Shape — •Fiona Berner, Chaurasia Rishi, Sajjad Shumaly, Chirag Hinduja, Hans-Jürgen Butt, and Rüdiger Berger — Max-Planck-Institut für Polymerforschung

The understanding of wetting phenomena plays a crucial role in many daily processes. For example, dirt repelling glasses can be achieved by a hydrophobic coating. Recently, Hinduja et al, reported on a scanning drop friction force instrument (sDoFFI) to analyse friction forces of drops on surfaces. A drop is fixated to an elastic force sensor with spring constant κ. The sample underneath the drop is moved with a constant speed u leading to sliding of the drop at a defined trajectory along surfaces. The deflection of the capillary,d, provides information about the friction force between the drop and the surface, $F_{meas} = \kappa \cdot d$ Forces arising from CAH are given by the Furmidge equation, where the drop*s sliding force F_{CAH} corresponds to

$$F_{CAH} = k \cdot \gamma \cdot w \cdot \big(cos(\theta_{rec}) - cos(\theta_{adv})\big) \qquad (1)$$

where k is a geometrical factor, γ is the liquid surface tension, w the width of the drop and θ_{rec} and θ_{adv} are the receding and advancing contact angles, respectively. For small u we assume $F_{meas} = F_{CAH}$. The parameters γ, w, θ_{rec} and θ_{adv} are known or can be measured optically. Thus, the geometrical factor k can be calculated. We realize different geometries of the drop by glueing metal rings to the elastic glass capillary. Shaping the metal rings forces the drop to shape. We discuss experiments where we shape the drop into different width and length and discuss dependence of the geometrical factor k.

CPP 9: French-German Session: Simulation Methods and Modeling of Soft Matter I

Time: Monday 15:00–17:00 Location: ZEU/LICH

Invited Talk CPP 9.1 Mon 15:00 ZEU/LICH

Why Polymers Swell or Collapse: Molecular Insights into Cosolute Effects — •Nico van der Vegt — Department of Chemistry, Technical University of Darmstadt

Water-soluble amphiphilic polymers are widely used as stimuli-responsive materials. Their performance is governed by the coil-globule transition, characterised by the theta temperature, which can be tuned by adding small organic molecules (cosolutes). Although related phenomena - such as cononsolvency and salting-out - are well understood at a phenomenological level, their underlying molecular mechanisms remain unclear. This talk explores the solvation physics that determine how different classes of cosolutes influence the coil-globule transition of both generic hydrophobic polymers and realistic systems such as poly(N-isopropylacrylamide), using computer simulations. We identify two distinct molecular driving forces that regulate cosolute-induced hydrophobic interactions, leading to either polymer swelling or collapse. These driving forces depend sensitively on the relevant length scales and expose the interplay between microscopic and macroscopic solvation physics, underscoring the key role of solvent entropy in determining the properties of responsive soft-matter systems. [1] Comm. Chem. 3, 165 (2020), [2] PCCP 24, 2080-2085 (2022), [3] J. Chem. Phys. 160, 164902 (2024)

CPP 9.2 Mon 15:30 ZEU/LICH

THz Pump Pulse Drives Nonlinear H-bond Dynamics in Liquid Water — •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

Light-matter interactions are central to processes in nature, chemical engineering, and fundamental research. Of particular interest is the frequency-dependent excitation of molecular systems by incident light. Here, we present machine-learning-accelerated molecular dynamics simulations of water subjected to an intense, monochromatic THz pump pulse, generating a total of 32 ns of trajectory data. The light pulse is explicitly modeled via a time-dependent external electric field, extending our previous framework for field-driven machine learning MD simulations, allowing us to observe the excitation in realtime. Our simulations reproduce key experimental observables, including transient dichroism and birefringence, and reveal that the pulse transiently modulates hydrogen-bond dynamics: H-bonds become markedly shorter-lived compared to unperturbed bulk water. This response is nonlinear, ruling out pure heating and resolving the experimental controversy. These results demonstrate that our machinery to incorporate electric fields in machine learning MD simulations can directly connect microscopic dynamics with measurable observables, further paving the way to controlling water dynamics - and potentially chemical reactivity - through tailored light pulses, a long-standing goal in chemistry.

CPP 9.3 Mon 15:45 ZEU/LICH

Fluctuating Solvent Fields and Vibrational Shifts Revealed by Machine Learned Force Fields — •Florian Brünig and Alexandre Tkatchenko — Department of Physics and Materials Science, University of Luxembourg, Luxembourg

Fluctuating solvent fields is one of the driving mechanism behind vibrational shifts observed in solvatochromic experiments [1]. Previously, experimental infrared spectra have been correlated with mean electric fields obtained from empirical force field molecular dynamics simulations [2]. However, vibrational dynamics of these force fields are insufficient to reproduce the experimental line shape properties.

Here, machine learned force fields (MLFFs) offer multiple opportunities: they are highly accurate, efficient, and can be interpretable if based on physical models. We explore the capabilities of modeling solvatochromism of vibrational probes in solvent and protein environments employing the SO3LR [3] MLFF. SO3LR combines the SO3krates architecture with pairwise analytical electrostatic and dispersion potentials in the long range, and was pretrained on a diverse data set of molecular complexes. We show how fluctuating solvent electrostatic and dispersion fields can be related to vibrational bands in a self consistent manner due to the versatility of MLFFs.

[1] Brünig, FN, Netz, RR, et al. JPCB 126, 1579 (2022).

[2] Weaver, JB, Kozuch, J, Kirsh, JM & Boxer, SG. JACS 144, 7562 (2022).

[3] Kabylda, A, Frank, JT, Müller, KR, Tkatchenko A, et al. JACS 147, 33723 (2025).

CPP 9.4 Mon 16:00 ZEU/LICH

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

Most Machine-Learning Potentials (MLPs) currently in use are local, which prevents the construction of accurate potentials for systems in which long-range charge transfer is important. One example is the distinction of different oxidation states of transition metal ions such as ferrous (Fe^{2+}) and ferric (Fe^{3+}) ions in aqueous solution. In this case the near-sightedness of local MLPs cannot account for distant counter ions or non-local charge transfer. We show that 4th-Generation High-Dimensional Neural Network Potentials (4G-HDNNPs), which employ atomic charges obtained from charge equilibration as globally-determined descriptors, do not suffer from this short-coming. For aqueous ferric and ferrous chloride, the model predicts iron oxidation states correctly matching the total number of chloride ions in the system demonstrating that physical knowledge about the system of interest remains essential to construct reliable MLPs.

CPP 9.5 Mon 16:15 ZEU/LICH

Bridging Accuracy and Sampling: Insights into dAMP Solvation from ML-potentials — •Laurie Stevens[1,2], Riccardo Martina[2], Alberta Ferrarini[2], and Marialore Sulpizi[1] — [1]Chair of Theoretical Physics of Electrified Liquid-Solid Interfaces, Faculty of Physics and Astronomy, Ruhr-Universität Bochum, Germany — [2]Department of Chemical Sciences, Università degli Studi di Padova, Italy

Although nucleotides are essential biomolecular building blocks, key aspects of their structure and interactions, in particular the steps enabling their assembly and polymerization, remain unclear. Here, we investigate the conformational behavior of deoxyadenosine monophosphate (dAMP) in solution using a combined computational-experimental approach. We developed a highly accurate machine-learning potential via active learning that thoroughly samples the free-energy landscape, capturing critical conformational degrees of freedom with near-chemical accuracy. This potential enables nanosecond-scale simulations of water and nucleotides at a level previously inaccessible with hybrid DFT methods. We find that, in solution, dAMP accesses both anti and syn glycosidic conformations. We identify the anti and high anti conformers as the most stable ones, we show that they underlie the intensity variations observed in mid-IR experimental spectra.

CPP 9.6 Mon 16:30 ZEU/LICH

Fine-Tuning Unifies Foundational Machine-learned Interatomic Potential Architectures at ab intio Accuracy — •Christian Dressler, Jonas Hänseroth, Nawaz Qaisrani, and Aaron Flötotto — TU Ilmenau, Institute of Physics, Germany

Machine-learned force fields (MLFFs) have enabled ab initio quality molecular dynamics at speedups of several orders of magnitude. Foundation-model MLFFs, trained on extremely large and diverse datasets, aim to provide broadly transferable force predictions, yet their accuracy remains system-dependent. We investigate five state-of-the-art foundation models (MACE, GRACE, ORB, MATTERSIM, SEVENNET) and fine-tune them for seven chemically diverse systems.[1] Our results show that foundation models provide a useful baseline but still deviate significantly from AIMD. Fine-tuning consistently improves accuracy across all frameworks and yields predictions that closely match AIMD reference data, while also reducing performance differences between models. The final accuracy is largely independent of the underlying architecture. These findings suggest that, after fine-tuning, model choice is no longer the main bottleneck. Prioritizing inference speed and computational efficiency may therefore offer the greatest benefit for accelerating the practical use of ML-based interatomic potentials in materials modeling.

[1] Hänseroth, ... , Dreßler, Fine-Tuning Unifies Foundational

Machine-Learned Interatomic Potential Architectures at ab initio Accuracy, https://doi.org/10.48550/arXiv.2511.05337

CPP 9.7 Mon 16:45 ZEU/LICH

NMR crystallography at finite temperatures — •Matthias Kellner and Michele Ceriotti — Laboratory of Computational Science and Modeling, Institut des Matériaux, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

In this talk I will present our latest developments in machine-learning models for predicting NMR chemical shieldings in organic molecular solids. NMR shielding-driven structure determination protocols rely on comparing experimental solid-state NMR shifts with simulations whose accuracy is often limited by computational cost. We address these limitations by combining ensembles of transformer-based shielding predictors with molecular dynamics simulations using a novel, broadly applicable machine-learning interatomic potential. This framework systematically improves agreement with experiment across many benchmark systems, removes the need for empirical corrections and makes it applicable also to disordered and amorphous materials. I will conclude by showing applications of this framework to the structure determination of amorphous active pharmaceutical ingredients.

CPP 10: Droplets, Wetting, and Microfluidics (joint session DY/CPP)

Time: Monday 15:00–18:30 Location: ZEU/0118

CPP 10.1 Mon 15:00 ZEU/0118

Rayleigh instability in the presence of elastocapillarity — •Niphredil Klint and Andreas Isacsson — Chalmers University of Technology, Gothenburg, Sweden

A liquid jet, such as a stream of water, will disintegrate and form droplets if the length-to-radius ratio exceeds a critical value. This occurs due to propagating surface instabilities, a phenomenon known classically as the Rayleigh instability. At the nanoscale, thermal fluctuations affect the breakup dynamics, which may enter a stochastic regime [1]. Placing an elongated nanoscale liquid drop with a high aspect ratio on top of a highly compliant surface, the breakup process is affected by additional noise from thermally excited flexural phonons [2] as well as effects whereby the wetting causes the underlying surface to deform. We use large scale molecular dynamics (MD) simulations to examine the dynamics of the Rayleigh instability in the presence of elastocapillary effects at ambient temperatures. Specifically, we study the interactions between water and suspended graphene, where wetting induced deformations may occur for nanoscale droplets [3]. We focus on characterising the breakup and instability wavelength and isolate the effects of introducing graphene through a comparison of these results to simulations of only water. We also identify the correlation between out-of-plane fluctuations of the graphene and the concentration of water.

[1] J. Eggers, Phys. Rev. Lett. 89, 084502 (2002).
[2] M. Ma et al., Nature Mater. 15, 66 (2016).
[3] M. Kateb et al, Langmuir 39, 12610 (2023).

CPP 10.2 Mon 15:15 ZEU/0118

Air layers and wetting under drops impacting on pre-wetted surfaces — •Kirsten Harth and Shiva Moradimehr — Fachbereich Technik, Technische Hochschule Brandenburg, Germany

Drop impact at low Weber numbers causes the formation of a (temporary) air cushion between the drop liquid and the substrate. On hard, dry substrates, its qualitative thickness profile and the location of the thinnest point are strongly governed by the Weber number. For impact on bulk, soft surfaces, like PDMS gels, it was found that impacts on softer substrates entrap more air [1]. Are there similar effects of thin liquid films?

We address the air layer shapes, entrapped air volume and wetting underneath droplets impacting on a hard substrate pre-wetted by microscopic oil layers. We control the Weber number, the oil layer thickness (in the range of micrometers), the oil viscosity, and in that way the *softness* of the substrate. Despite the thinness of the film, we observe clear effects of the oil layer on the volume and drainage of the air entrapment, its profile shapes, and the wetting behavior.

[1] K.R. Langley et al., Soft Matter 16, 5702 (2020)

We acknowledge funding by DFG within SPP2171 (HA8467/2-1, 2-2).

CPP 10.3 Mon 15:30 ZEU/0118

Memory Effects in Contact Line Friction — •Niklas Wolf and Nico van der Vegt — TU Darmstadt, Darmstadt, Germany

When a drop of liquid comes into contact with a solid surface, it relaxes towards an equilibrium configuration, either wetting the surface or remaining in a droplet-like shape with a finite contact angle. The speed of this relaxation strongly depends on a friction force opposing the movement of the three-phase contact line. In analogy to the treatment of hydrodynamic friction we present an exact method, based on the Mori-Zwanzig formalism, to extract this friction from equilibrium data. Within the linear response regime, we obtain the frequency-dependent dissipative and elastic response of the contact line to an external perturbation, including a frequency-dependent friction coefficient. We find that the contact line exhibits long-lasting memory with a power-law decay due to coupling to the systems hydrodynamic modes. As a result the microscopic contact line dynamics are neither Markovian nor determined by the movement of a few molecules in the vicinity of the contact line.

CPP 10.4 Mon 15:45 ZEU/0118

Reaction-Mediated Arrest and Gradient-Driven Droplet Transport — •Stefan Köstler[1,2], Yicheng Qiang[1], Malcolm Steen[1,2], Guido Kusters[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

Controlling droplet size and position is central to many biological and engineering processes. Chemical reactions can arrest coarsening and sustain spatial concentration gradients, while hydrodynamic flows generally accelerate coarsening and drive droplets along chemical gradients. Using continuum theory, we show that the competition between reactions, diffusion, and hydrodynamic advection yields rich behavior even in binary systems: Advection dominates the coalescence of small droplets, diffusion leads to Ostwald ripening for intermediate sizes, and reactions finally suppress coarsening. Interestingly, a range of droplet sizes is stable, depending on initial conditions and the strength of advection. Crucially, chemical gradients can actively steer droplets and couple to size-control. Our results demonstrate practical routes to control both the size distribution and spatial organization of droplets by tuning chemical activity and gradient-driven flows.

CPP 10.5 Mon 16:00 ZEU/0118

From bipedal to chaotic motion of chemically fueled partially wetting liquid drops — •Florian Voss[1] and Uwe Thiele[1,2] — [1]Institute of Theoretical Physics, University of Münster — [2]Center for Data Science and Complexity (CDSC), University of Münster

Chemomechanical coupling is essential to various phenomena in soft matter systems that are kept permanently out of thermodynamic equilibrium, e.g., in reactive complex liquids. Based on a thermodynamically consistent continuum model, we demonstrate that partially wetting liquid drops covered by chemically reacting surfactants display a variety of biomimetic motility modes like shuttling, bipedal, rotational and quasi-random motion when supplied with chemical fuel from an ambient bath. The dynamics originates from chemomechanical feedback between the reaction network on the drop and the Marangoni effect [1] and becomes increasingly complex as a result of competing length scales. Due to the generic underlying thermodynamic structure, we expect that our results are also relevant for other chemically active mixtures and soft matter systems.

[1] F. Voss and U. Thiele, Phys. Rev. Fluids 10, 94005 (2025).

CPP 10.6 Mon 16:15 ZEU/0118

Odd Droplets — •Thomas Appleford — University of Amsterdam, Amsterdam, Netherlands

In chiral systems such as active spinning colloidal matter, time-reversal symmetry-breaking interactions often give rise to a macroscopic continuum description in which the stress tensor contains off-diagonal terms. In fluids, these off-diagonal components lead to so-called "odd-viscous" deformations, in which energy is not dissipated. Odd viscous fluids have been shown to exhibit a rich variety of phenomena, including symmetry-broken flow around translating droplets and asymmetric droplet spreading on superhydrophobic surfaces. Our work investigates the behaviour of droplets in suspension. In particular, we present an analytical solution to the droplet-in-shear problem within the framework of two-dimensional odd Stokes flow, followed by the derivation of a formula for the apparent viscosity of a dilute emulsion. We then explore how chirality can be parametrically varied to tune the bulk rheological properties and control the system's overall energy dissipation.

CPP 10.7 Mon 16:30 ZEU/0118

Stretching and Sliding Capillary Bridges — •Lennard Holschuh and Lars Pastewka — University of Freiburg, Department of Microsystems Engineering

Capillary forces play a critical role in the adhesion between two contacting bodies. However, existing theories of macroscopic adhesion on rough surfaces often assume dry conditions, attributing adhesive interactions solely to dispersion forces and overlooking the effects of capillary bridge formation. This study employs molecular dynamics simulations to directly examine the interactions of nanoscale probes with nominally flat surfaces in the presence of liquid bridges, which form due to condensation in humid environments. The objective is to link the thermodynamic understanding of capillary bridges with molecular simulations and atomic-force microscopy experiments. These calculations focus on investigating energy dissipation during adhesion (normal separation of the probe from the surface) and friction (lateral motion of the probe). By quantifying the interplay between relative humidity, adhesion, and friction, this work aims to improve the understanding of macroscopic adhesion in humid conditions and guide the development of materials with tailored properties for high-precision applications, such as microelectronic manufacturing.

15 min. break

CPP 10.8 Mon 17:00 ZEU/0118

Hyperuniformity in Ternary Fluid Mixtures: The Role of Wetting and Hydrodynamics — •Nadia Bihari Padhan and Axel Voigt — Institute of Scientific Computing, TU Dresden, 01069 Dresden, Germany

Phase separation in multicomponent fluids underlies the organization of complex materials and biological structures, including biomolecular condensates. The Cahn-Hilliard-Navier-Stokes (CHNS) framework provides a natural description of such systems by coupling diffusive and hydrodynamic processes. In this talk, I will present our study of hyperuniformity–suppressed large-scale density fluctuations–in ternary CHNS mixtures. We show that hydrodynamics systematically drives the system toward less hyperuniform states and generates a rich set of morphologies, such as interconnected droplets and double emulsions reminiscent of biological phase separation. In partial-wetting regimes, all three components display comparable hyperuniformity, whereas in complete-wetting regimes the preferred wetting component exhibits a marked loss of hyperuniformity. These results identify wetting asymmetry as a key control parameter for spatial order in multiphase fluids and offer a pathway for tuning large-scale organization in soft-matter and biological systems.

References [1] Boyer, F. and Lapuerta, C., Study of a three component Cahn-Hilliard flow model, ESAIM: Mathematical Modelling and Numerical Analysis, 40, 653-687 (2006). [2] Padhan, Nadia Bihari and Voigt, Axel, Hyperuniformity in ternary fluid mixtures: the role of wetting and hydrodynamics, arXiv:2506.22647, (2025).

CPP 10.9 Mon 17:15 ZEU/0118

Effect of Flow Coupling on Defect Binding and Unbinding in Nematic Fluids — •Jayeeta Chattopadhyay, Simon Guldager Andersen, Kristian Thijssen, and Amin Doostmohammadi — Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, Copenhagen, Denmark.

Topological defects play a central role in the ordering and dynamics of nematic fluids. We investigate how coupling to fluid flow modifies defect-mediated phase transitions in two-dimensional nematics using fluctuating nematohydrodynamic simulations. The system is driven by tuning the fluctuation strength, with increasing and decreasing fluctuations defining forward and backward protocols. Without flow coupling, the system undergoes a Berezinskii–Kosterlitz–Thouless (BKT)–like transition via the reversible binding and unbinding of $\pm 1/2$ defect pairs. When hydrodynamics is included, the transition depends on the flow–alignment parameter: non-aligning nematics ($\lambda = 0$) retain BKT-like behavior, whereas strain-rate–aligning nematics ($\lambda \neq 0$) form bend–splay walls, lowering the defect-creation threshold and preventing recombination, leaving defects unbound across all fluctuation strengths. In active nematics, defects remain unbound for all λ, showing that self-generated flows also inhibit bound-pair formation. These results demonstrate that coupling to fluid flow fundamentally alters topological phase behavior, suppressing the equilibrium BKT binding mechanism.

CPP 10.10 Mon 17:30 ZEU/0118

Electrophoresis in charged chiral active fluids with odd viscosity — •Reinier van Buel, Bogdan Cichocki, and Jeffrey Everts — Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

Understanding the motion of colloidal particles dissolved in fluids that exhibit odd viscosity – a specific component of the viscous stress tensor found in e.g. chiral active fluids – is of particular interest for realising nontrivial particle transport and characterising out-of-equilibrium thermodynamic properties. Although three-dimensional odd viscosity has not yet been experimentally observed, charge stabilisation is expected to be vital in enabling such measurements. Therefore, we introduce the notion of a charged chiral active fluid and we investigate some of its non-trivial electrokinetic properties. In particular, we focus on electrophoresis of a charged sphere suspended in such an odd viscous fluid. Here, the peculiar nature of odd viscosity breaks the spherical symmetry of the system, and through coupling with the electric double layer and its screening properties, alters the electrophoretic mobility. Using the Lorentz reciprocal theorem, we derive expressions for the electrophoretic mobility of a spherical particle based on the analytical solution for the uncharged flow. Furthermore, we highlight how the Hückel and Smoluchowski limits of the electrophoretic mobility are affected by odd viscosity. Our results demonstrate that odd viscosity leads to directional asymmetries in the electrophoretic mobility tensor, suggesting mechanisms for active control of charged colloidal motion in systems where odd viscosity is prevalent.

CPP 10.11 Mon 17:45 ZEU/0118

Experimentally probing microscale torsional memory in a viscoelastic fluid — •Niloyendu Roy[1], Rupayan Saha[2], Debankur Das[2], Matthias Krüger[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Institut für Theoretische Physik, Universität Göttingen, Göttingen, Germany

Motion of a colloid inside viscoelastic fluids follows non-Markovian dynamics, meaning its trajectory is influenced by past motion. Such memory effects are typically attributed to intrinsic material timescales arising from relaxation of the fluid microstructure and are usually probed using translationally driven colloids. Here we show experimentally that rotational driving of a colloid by a controlled torque elicits a far richer form of memory: the relaxation of the resulting torsional stresses spans a broad distribution of timescales, even though the fluid itself possesses a single dominant relaxation time. This behaviour allows time-dependent torsional driving histories to be encoded and subsequently read out through characteristic non-monotonic recoil responses. By mapping the flow field and the spatial distribution of torsional stresses, we demonstrate that the geometry of rotation generates an orthogonality between the propagation of angular momentum and the storage of torsional stresses, producing a spatio-temporal memory field not accessible through translational forcing. These results establish torsional driving as a powerful route to generate, store, and retrieve memory in viscoelastic fluids, opening new possibilities for soft-matter information storage and torque-responsive microdevices.

CPP 10.12 Mon 18:00 ZEU/0118

3D Optofluidic Control Using Reconfigurable Thermal Barriers — •Falko Schmidt[1,2], Carlos David Gonzalez[3], Marc Sulliger[1], Emilio Ruiz-Rena[4], Raul A. Rica[3,5], Jaime Ortega-Arroyo[1], and Romain Quidant[1] — [1]Department of Mechanical and Process Engineering, ETH Zurich, Zurich 8092, Switzerland — [2]Peter Debye Insitute for Soft Matter Physics, Leipzig University, 04103 Leipzig, Germany — [3]Universidad de Granada, Department of Applied Physics, Granada 18071, Spain — [4]Department of Applied Physics

II, University of Malaga, Malaga 29071, Spain — [5]Universidad de Granada, Research Unit Modeling Nature (MNAT), Granada 18071, Spain

Optothermal manipulation enables precise control of small particles via optical and thermal forces, leveraging thermo-osmotic and convective flows for short- and long-range motion. We present a reconfigurable optofluidic method enabling diverse manipulations such as guiding, sorting, trapping, and separating particles. Using light absorption on plasmonic surfaces of gold nanorods, localized hot spots are generated, creating temperature-driven flows. A near-infrared laser spatially modulates temperature landscapes, monitored by 3D holographic microscopy and optical diffraction tomography. Single and double heat sources produce three-dimensional flow control. This creates an optofluidic barrier that redirects particles within a microfluidic chamber. This approach offers a versatile foundation for advancing microfluidic technologies, enabling applications in sorting, trapping, and adaptive system design.

CPP 10.13 Mon 18:15 ZEU/0118

Dynamics and Ordering of Microdroplets in Marangoni Flow Field — •Akshay Kallikkunnath and Frank Cichos — Molecular Nanophotonics, Peter Debye Institute for Soft Matter Physics, Faculty of Physics and Earth System Sciences, Leipzig University, Linnéstraße 5, 04103 Leipzig, Germany

Collective organization and internal dynamics are intimately linked and emerge across biological scales, with ordered structures providing a framework within which individual constituents remain dynamically active. Here, we study a system of water-in-oil microdroplets containing heat-releasing particles that organize under thermally induced flows. A sub-kelvin temperature increase from the heated particle at the air-oil interface generates Marangoni circulation that advects the droplets. Interactions through the flow field lead to robust ordering, while internal particle dynamics reflect coupling between local thermal gradients and microscale hydrodynamics. This provides a controllable platform to probe self-organization and emergent order by generating flows driven by weak, localized thermal fields in a fully fluid-in-fluid environment.

CPP 11: Active Matter II (joint session DY/BP/CPP)

Time: Monday 15:00–18:30 Location: ZEU/0160

CPP 11.1 Mon 15:00 ZEU/0160

Field-controlled self-organization in an active spin system — Mintu Karmakar[1,2,3], •Matthieu Mangeat[4], Swarnajit Chatterjee[5,4], Heiko Rieger[4], and Raja Paul[3] — [1]WIUCAS, Beijing, China — [2]Universitat de Barcelona, Barcelona, Spain — [3]IACS, Kolkata, India — [4]Saarland University, Saarbrücken, Germany — [5]CY Cergy Paris Université, Cergy-Pontoise, France

We investigate the collective response of active Potts particles to an external magnetic field and uncover three striking nonequilibrium phenomena. We first examine how the flocking transition is reshaped for a homogeneous and unidirectional field: the coexistence regime between an apolar gas and a polar liquid is replaced by a phase separation between two polar-ordered phases, a low-density, weakly polarized background and a high-density, strongly polarized band, both moving along the field. Second, when the particles self-organize into a high-density longitudinal lane whose long axis is perpendicular to the field, the lane slowly treadmills against the field direction, driven by the weakly polarized background. Finally, we identify a field-induced interface pinning regime that arises when the domain is divided into two regions with opposite field directions, causing particles to accumulate and perform a back-and-forth motion at the interface. This pinning phenomenon also leads to the emergence of a disordered state in the presence of a random field orientation. A coarse-grained hydrodynamic theory supports and confirms the phenomena observed in our microscopic simulations.

CPP 11.2 Mon 15:15 ZEU/0160

Nucleation kinetics in two-dimensional polar active fluids — •Yuta Kuroda and Thomas Speck — Institute for Theoretical Physics IV, University of Stuttgart, Germany

Polar active fluids constitute one of the most important classes of active matter. These systems possess alignment interactions that cause the local polarization to align with that of neighboring particles, leading to a flocking transition in which global polar order emerges. Extensive numerical and analytical studies have established that the flocking transition is discontinuous, and consequently, the phase diagram possesses a coexistence region in which propagating polar bands appear. Despite intensive studies on flocking transitions, the nucleation mechanism responsible for the formation of these bands remains poorly understood. In this work, we numerically investigate the nucleation kinetics of polar bands using a particle model, namely active Brownian particles with a Kuramoto-type alignment interaction, and we report the behavior of the nucleation rate over a wide range of parameters.

CPP 11.3 Mon 15:30 ZEU/0160

Collision dynamics of active Brownian hard disks — •Jonas Buba — Soft Matter Theory Group, Theoretical Physics: Lab for Emergent Phenomena, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Active matter systems, composed of self-driven agents, display emergent behaviors such as collective motion, clustering, and motility-induced phase separation (MIPS). To better understand the microscopic origin of MIPS, we study collisions of active Brownian hard disks within the framework of dynamical density functional theory (DDFT). The particle interactions are modeled using fundamental measure theory (FMT). Each particle is represented by a Gaussian density peak, which allows us to quantify the mean delay from collisions for different configurations. The post-collision density resulting from the simulation can be described by a convolution of the pre-collision density, enabeling the analysis of different contributions to the delay.

CPP 11.4 Mon 15:45 ZEU/0160

Active Ornstein-Uhlenbeck Particles: A Stochastic Path Integral Approach — •Carsten Littek, Mike Brandt, and Falko Ziebert — Institut für Theoretische Physik, Universität Heidelberg, Germany

In a recent publication (arXiv:2509.26296) we have developed a path integral formulation of the stochastic dynamics of a single active Brownian particle (ABP), with or without a constant torque, confined by a harmonic trap. This approach is based on the particle's microscopic degrees of freedom and we have derived exact analytic time-dependent expressions for key observable quantities such as the mean position and mean square displacement without the necessity of solving the Fokker-Planck equation. Here we present the application of this approach to the dynamics of active Ornstein-Uhlenbeck particles (AOUP). In particular, we generalize our formulation to systems of many AOUPs interacting via a suitable two-particle potential and derive the statistical quantities relevant in the context of collective phenomena, such as motility-induced phase separation (MIPS).

CPP 11.5 Mon 16:00 ZEU/0160

Self-alignment and chirality in dense active matter: from flocking to circling crystals — •Marco Musacchio[1], Alexander Antonov[1], Hartmut Löwen[1], and Lorenzo Caprini[2] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany — [2]Physics Department, University of Rome La Sapienza, P.le Aldo Moro 5, IT-00185 Rome, Italy

Several experimental systems in active matter are characterized, at the single-particle level, by an effective torque that aligns particle orientation with their instantaneous velocity. This mechanism, known as self-alignment, appears in both biological and granular active systems. In dense active systems, a sufficiently strong self-alignment can suppress mips and drive the system from a clusterized flocking state to an homogeneous one, where all particles move collectively, with aligned velocities. This flocking transition is approached for a broad range of densities, even close to maximal packing, where the system is in a crystalline configuration. Specifically, in the crystal case, the flocking transition can be predicted analytically since the dynamics can be mapped onto a velocity-dependent Landau*Ginzburg free energy, revealing that this disorder*order transition is second order. The onset of chirality drives the system from collective flocking to a circling crystal phase, characterized by coherent circular motion of all the system. Further increasing chirality suppresses the global rotation, leading to a vortex-like structure in the velocity field. These findings are experimentally testable in systems governed by self-alignment and chirality.

CPP 11.6 Mon 16:15 ZEU/0160

Number fluctuations distinguish different self-propelling dynamics — •Tristan Cerdin[1,2], Sophie Marbach[2], and Carine Douarche[1] — [1]Université Paris-Saclay, CNRS, FAST, 91405, Orsay, France — [2]CNRS, Sorbonne Université, Physicochimie des Electrolytes et Nanosystèmes Interfaciaux, F-75005 Paris, France

In nonequilibrium suspensions, static number fluctuations N in virtual observation boxes reveal remarkable structural properties, but the dynamic potential of $N(t)$ signals remains unexplored. Here, we develop a theory to learn the dynamical parameters of self-propelled particle models from $N(t)$ statistics.

Theoretical plots of the mean-squared number difference $\langle \Delta N^2(t) \rangle$ exhibit 3 scaling regimes in time corresponding to the 3 regimes of self-propelled particles: diffusive, advective and effectively diffusive again at long times. By expanding the theory in each of these regimes, we recover limiting laws for the number fluctuations, which can be used in practice to quantify self-propulsion properties.

Additionally, unlike traditional trajectory analysis, $N(t)$ statistics distinguish between models, by sensing subtle differences in reorientation dynamics that govern re-entrance events in boxes. This paves the way for quantifying advanced dynamic features in dense, out-of-equilibrium suspensions.

CPP 11.7 Mon 16:30 ZEU/0160

Flocking transitions in dense mixtures of active self-aligning and passive particles — •Weizhen Tang[1], Amir Shee[2], Zhangang Han[1], Pawel Romanczuk[3,4], Yating Zheng[3,4], and Cristián Huepe[1,5,6] — [1]School of Systems Science, Beijing Normal University, Beijing, China — [2]Department of Physics, University of Vermont, USA — [3]Department of Biology, Humboldt Universität zu Berlin, Unter den Linden 6, Berlin, Germany — [4]Research Cluster of Excellence 'Science of Intelligence', Berlin, Germany — [5]Northwestern Institute on Complex Systems and ESAM, Northwestern University, Evanston, USA — [6]CHuepe Labs, 2713 West Augusta Blvd #1, Chicago, USA

We investigate the passivity-driven flocking transition in a dense mixture of self-aligning active particles and passive particles, using a minimal model of active polar disks. We show that anisotropic damping leads to a discontinuous flocking transition as a function of the fraction of passive components, whereas isotropic damping produces a smooth transition where the final ordered state can display sustained oscillations and remain trapped in a metastable state, depending on the exact spatial arrangement of the passive particles. We also explore in detail the emergence of metastable oscillatory ordered states and their relation to the spatial distribution of passive particles and interstitial voids. Our findings demonstrate that heterogeneous activity and mobility anisotropy can result in a rich variety of self-organized states in various biological systems, synthetic active materials, and robotic swarms.

15 min. break

Invited Talk CPP 11.8 Mon 17:00 ZEU/0160

Topological transition in filamentous cyanobacteria: from motion to structure — •Marco Mazza — Loughborough University, Loughborough, UK

Many active systems are capable of forming intriguing patterns at scales significantly larger than the size of their individual constituents. Cyanobacteria are one of the most ancient and important phyla of organisms that has allowed the evolution of more complex life forms. Despite its importance, the role of motility on the pattern formation of their colonies is not understood. Here, we investigate the large- scale collective effects and rich dynamics of gliding filamentous cyanobacteria colonies, while still retaining information about the individual constituents' dynamics and their interactions. We investigate both the colony's transient and steady-state dynamics and find good agreement with experiments. We furthermore show that the Péclet number and aligning interaction strength govern the system's topological transition from an isotropic distribution to a state of large-scale reticulate patterns. Although the system is topologically non-trivial, the parallel and perpendicular pair correlation functions provide structural information about the colony, and thus can be used to extract information about the early stages of biofilm formation. Finally, we find that the effects of the filaments' length cannot be reduced to a system of interacting points. Our model proves to reproduce both cyanobacteria colonies and systems of biofilaments where curvature is transported by motility.

CPP 11.9 Mon 17:30 ZEU/0160

Novel Phase Coexistence in a Multi-Species Vicsek Model — •Eloise Lardet[1], Letien Chen[1,2], and Thibault Bertrand[1] — [1]Imperial College London, UK — [2]University of Edinburgh, UK

A hallmark in natural systems, self-organization often stems from very simple interaction rules between individual agents. While single-species self-propelled particle (SPP) systems are well understood, the behavior of mixtures of self-propelled particles with general alignment interactions remains largely unexplored with a few scattered results hinting at the existence of a rich emergent phase behavior. Here, we first present a generalization of the two-species Vicsek model with reciprocal intra- and interspecies (anti-)alignment couplings, uncovering a rich phenomenology of emergent states. Notably, we show that rather than destroying polar order, anti-aligning interactions can promote phase separation and the emergence of global polar order. Secondly, we derive a kinetic theory for the system, finding good agreement between theoretical predictions and particle simulations. This includes a novel mechanism for microphase separation, as predicted by a Turing instability. We finally show that these coexistence patterns can be generalized to multi-species systems with cyclic alignment interactions.

CPP 11.10 Mon 17:45 ZEU/0160

Flocking in weakly nonreciprocal mixtures — •Charlotte Myin — Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Goettingen, Germany

We show that weakly nonreciprocal alignment leads to large-scale structure formation in flocking mixtures. By combining numerical simulations of a binary Vicsek model and the analysis of coarse-grained continuum equations, we demonstrate that nonreciprocity destabilizes the ordered phase formed by mutually aligning or anti-aligning species in a large part of the phase diagram. For aligning populations, this instability results in one species condensing in a single band that travels within a homogeneous liquid of the other species. When interactions are anti-aligning, both species self-assemble into polar clusters with large-scale chaotic dynamics. In both cases, the emergence of structures is accompanied by the demixing of the two species, despite the absence of repulsive interactions. Our theoretical analysis allows us to elucidate the origin of the instability, and show that it is generic to nonreciprocal flocks.

CPP 11.11 Mon 18:00 ZEU/0160

Collective behavior in nonreciprocal multi-species Vicsek model with permutation symmetry — •Jae Dong Noh[1], Chul-Ung Woo[2], and Heiko Rieger[2] — [1]Department of Physics, University of Seoul, Seoul 02504, Korea — [2]Department of Theoretical Physics and Center for Biophysics, Saarland University, Saarbrücken, Germany

Nonreciprocal systems are typically built upon asymmetric roles among interacting agents, such as a pursuer-evader relationship. We propose a multi-species nonreciprocal active matter model that is invariant under permutations of the particle species. The nonreciprocal, yet symmetric, interactions emerge from a constant phase shift in the velocity alignment interactions, rather from an asymmetric coupling matrix. This system displays rich collective behaviors, including a species-mixed chiral phase with quasi-long-range polar order and a species-separated vortex cell phase. We present numerical evidence for these phases using particle-based Monte Carlo simulations and analytic evidence using continuum Boltzmann and hydrodynamic equations. Our work demonstrates that multi-species chiral fluids can be realized by a nonreciprocal but symmetric alignment interaction, where the rich collective behavior is a consequence of the interplay between nonreciprocity and permutation symmetry.

CPP 11.12 Mon 18:15 ZEU/0160

Flocking with random non-reciprocal interactions — •Jiwon Choi[1], Jae Dong Noh[2], and Heiko Rieger[1] — [1]Department of Physics & Center for Biophysics, Saarland University, Campus E2 6, 66123 Saarbrücken, Germany — [2]Department of Physics, University of Seoul, Seoul, 02504, Korea

Flocking is ubiquitous in nature and emerges from alignment interactions among self-propelled agents. Two species that anti-align or interact non-reciprocally exhibit complex collective phenomena, ranging from parallel and anti-parallel flocking and run-and-chase behavior to chiral phases. Whether such behavior survives in the presence of many species with random non-reciprocal interactions has remained unclear. As a first step, we study a continuous-time Vicsek-like model with fully random non-reciprocal interactions between particles. For infinite-range interactions, flocking emerges once the alignment bias becomes comparable to the non-reciprocal interactions, and deep inside this phase random non-reciprocity can still support slow global chiral and oscillating states. For short-range interactions, even without alignment bias, self-organized cliques form, where medium-sized clusters with predominantly aligning interactions remain stable over long times. We further investigate the robustness of clique formation and the coexistence phase under angular noise using a discrete-time Vicsek model with random non-reciprocal interactions. These results provide a basis for studying multi-species flocking with complex non-reciprocal interactions.

CPP 12: French-German Session: 2D Materials, Thin Films and Interfaces I

Time: Monday 15:00–17:00 Location: ZEU/0255

Invited Talk CPP 12.1 Mon 15:00 ZEU/0255

Multifunctional films by tailoring chemistry and morphology of polymer brushes at the nanoscale — •Petra Uhlmann and Alexander S. Münch — Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, 01069 Dresden

Functional polymer thin films, like stimuli-responsive polymer brushes or cross-linked polymer networks, are a group of smart surface coatings which are beneficial for the design of intelligent interfaces. One emphasis of our work is the synthesis of polymer brushes as a toolbox for the creation of specific surface functions and stimuli-responsive layers using a bottom-up approach. For many technical applications control and switching of wettability is a key property. In this contribution it will be shown how tailored co-polymers containing zwitterionic phosphorylcholine groups (MPC) and benzophenone (BPO) as anchoring and UV cross-linking units can be used to create multifunctional films with easy-to-clean, anti-fog, anti-fouling and anti-icing properties. For the achievement of the desired surface functions the control of not only the wettability, but also other thin film properties like thickness and degree of swelling, are crucial and require the respective optimization of the chemical polymer composition and the degree of crosslinking. For verification and adjustment of the interfacial and thin film properties atomic force microscopy (AFM), infrared spectroscopy (ATR-FTIR), contact angle measurements, and in-situ spectroscopic ellipsometry were used and correlated with respective coatings performance and sustainability tests.

CPP 12.2 Mon 15:30 ZEU/0255

Increase in elastic modulus of thin elastic films and membranes containing rigid inclusions - revisiting Einstein's relation in two dimensions — •Konstantin Zisiadis and Andreas Menzel — Otto-von-Guericke-Universität Magdeburg

Elastic matrices with well-separated inclusions can be described by effective elastic moduli obtained via homogenization methods. Probably the most basic relation for dilute systems is the Einstein equation $\eta_{\mathrm{eff}} = \eta(1 + 2.5\phi)$. We consider the two-dimensional geometry of an elastic matrix in two dimensions with two-dimensional elastic moduli as counterparts to the three-dimensional case. Both plane-stress and plane-strain geometries are treated. We employ a generalized stresslet formalism. Our derived formulae for the effective moduli of the two-dimensional geometry are expressed using the two-dimensional elastic moduli for an arbitrarily compressible matrix. We find that the plane-stress and plane-strain equations for the effective moduli have the same form, while the associated two-dimensional moduli differ. Our results are consistent with previous research based on different approaches. For an incompressible matrix, we recover the known effective shear modulus $\mu_{\mathrm{eff}} = \mu(1 + 2\phi)$.

We acknowledge support by the German Research Foundation (DFG) through Research Unit FOR 5599 on structured magnetic elastomers.

CPP 12.3 Mon 15:45 ZEU/0255

Structure and optical properties of donor-HATCN blends — •Gianfranco Melis, Dmitry Lapkin, Ainur Abukaev, Alexander Hinderhofer, and Frank Schreiber — Universität Tübingen, Tübingen, Germany

Organic thin films made of molecular semiconductors have the potential to advance the range of functional materials for technological progress. In this regard, electron donor-acceptor complexes (DAC) show unique physical properties at specific ratios due to their non-linear structure-property-composition dependence. A systematic study across the full mixing range is therefore essential to understand how structure and optical response evolve with composition.

Compositional-gradient thin films were prepared in a custom-built organic molecular beam deposition chamber by co-depositing donor materials—diindenoperylene (DIP), pentacene (PEN), coronene (COR), picene (PIC), α-sexithiophene (α-6T), zinc phthalocyanine (ZnPc), and perylenetetracarboxylic acid bis(propylimide) (PTCDI-C_3)—with the prospective non-fullerene acceptor hexaazatriphenylenehexacarbonitrile (HATCN). Grazing-incidence wide-angle X-ray scattering (GIWAXS), atomic force microscope (AFM), and UV-Vis absorption spectroscopy were applied to study and correlate structural and optical properties with the donor-acceptor stoichiometry. New absorption bands appear below the optical bands of pure materials at specific stoichiometric compositions, together with different surface morphologies and the formation of new mixed structural phases.

CPP 12.4 Mon 16:00 ZEU/0255

Optimized Phenyl-Modified g-C3N4/ZnO Hybrid Thin Films: Structural and Optical Insights — •Sahar Aghapour Ghourichay[1,2], Morgan Le Du[2], David P. Kosbahn[2], Guangjiu Pan[2], Hagen Uebele[2], Thomas Baier[2], Jinsheng Zhang[2], Lyuyang Cheng[2], Pier Carlo Ricci[1], and Peter Müller-Buschbaum[2] — [1]Department of Physics, University of Cagliari, Cittadella Universitaria, Monserrato, Italy — [2]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Phenyl-modified graphitic carbon nitride (PhCN)/ZnO hybrid thin films were fabricated with different PhCN loadings to investigate the influence of interface engineering on their structural and optical properties. UV-vis reflectance results show that the film containing 1 mL PhCN exhibits the lowest reflectance and the strongest absorption in the visible region. Photoluminescence analysis confirms that this optimized film has significantly reduced emission intensity, indicating more effective charge separation. XRD, AFM, and GIWAXS measurements reveal improved crystallinity and enhanced nanoscale ordering of ZnO in the presence of moderate PhCN content. SEM/EDS mapping verifies uniform hybrid formation, and XPS provides evidence of interfacial chemical interaction. Overall, controlled PhCN incorporation effectively tunes the optical response and nanoscale structure of PhCN/ZnO thin films, offering useful insights for photocatalytic and optoelectronic applications.

CPP 12.5 Mon 16:15 ZEU/0255

Machine Learning for Grazing-Incidence Diffraction (GID): from Raw Data to Crystalline Structure — •Dmitry Lapkin, Ainur Abukaev, Ekaterina Kneschaurek, Mikhail Romodin, Constantin Völter, Vladimir Starostin, Alexander Hinderhofer, and Frank Schreiber — Universität Tübingen

The optimization of novel materials in the form of thin films for specific applications requires the appropriate structural characterization methods. X-ray and neutron scattering techniques, such as grazing incidence small- and wide-angle X-ray/neutron scattering (GISAXS/GIWAXS/GISANS) or grazing-incidence diffraction (GID), offer the ultimate spatial resolution and high surface sensitivity, making them indispensable tools for thin film studies. At the same time, advancements in X-ray and neutron sources, in conjunction with developments in area detector technologies, enable the recording of several terabytes of raw two-dimensional detector data within a single experiment. Conventional methods of analyzing the GID data are severely under-paced compared to the data generation rates, representing a significant bottleneck and leaving much of the measured data unanalyzed. To make the thin film studies more efficient and increase the amount of analysed and published GID data that can be reused, we are developing a comprehensive machine learning based data analysis pipeline that goes from raw detector patterns to the corresponding crystalline structures. This pipeline comprises several stages, including data preprocessing and reduction, Bragg peak identification and refinement, and crystal structure determination.

Invited Talk CPP 12.6 Mon 16:30 ZEU/0255

Thin-film and interface properties in energy conversion devices unveiled by X-rays — •Marcus Bär — Department Interface Design, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), Berlin, Germany — Energy Materials In-Situ Laboratory Berlin, HZB, Berlin, Germany — Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — Department of X-ray Spectroscopy at Interfaces of Thin Films, Helmholtz-Institute Erlangen-Nürnberg for Renewable Energy, Berlin, Germany

This invited talk will present recent advances in the characterization of the chemical and electronic structure of interfaces and thin films that are central to modern energy-conversion technologies. A combination of X-ray spectroscopies enables non-destructive, depth-resolved insight into composition, chemical structure as well as bonding and energy-level landscapes across complex and often (deeply) buried interfaces. Interfacial intermixing, interlayer formation, oxidation processes, and energy-level alignment govern charge transport and recombination in energy conversion materials and devices. Illustrative case studies will be used to demonstrate how changes (e.g., in the thin-film deposition process) affect interfacial chemistry and electronic structure, highlighting the importance of the ability to probe interface properties as a prerequisite for deliberate interface design. In addition, the talk will outline recent progress in establishing dedicated sample environments allowing for in-situ and operando studies opening new pathways for understanding dynamic interface phenomena.

CPP 13: Charged Soft Matter, Polyelectrolytes and Ionic Liquids

Time: Monday 15:00–17:00 Location: ZEU/0260

Invited Talk CPP 13.1 Mon 15:00 ZEU/0260

Modelling and simulation of pH-sensitive polyelectrolyte microgels — •Stefanie Schneider — Institute of Physical Chemistry, RWTH Aachen University, Aachen, Germany

For weak polyelectrolytes (PE) as well as for weak polyampholytes (PA), not only the pH-pKA value but also the local electrostatic environment of the ionisable group determines the degree of ionisation and structural properties of the polymer. The proximity of already ionised groups, which is enforced by the interconnectivity of the polymer chain, influences the probability of additional groups to become ionised. Therefore, the degree of ionisation for polymers with different architectures differs from the ideal value, obtained for monomers at low concentrations.

Polyelectrolyte and polyampholyte microgels of different topologies have been investigated using constant pH-Monte Carlo simulations. Ionisation, swelling as well as the uptake and release of guest molecules were studied. [1-5]

Especially, the interaction with guest molecules is an important aspect for the use of microgels for drug delivery.

[1] C. Hofzumahaus, P. Hebbeker, S. Schneider, Soft Matter, 2018, 14, 4087.

[2] C. Hofzumahaus, C. Strauch, S. Schneider, Soft Matter, 2021, 17, 6029.

[3] C. Strauch, S. Schneider, Soft Matter, 2023, 19, 938.

[4] C. Strauch, S. Schneider, Soft Matter, 2024, 20, 1263.

[5] C. Strauch, L. Roß, S. Schneider, Soft Matter, 2024, 20, 9664.

CPP 13.2 Mon 15:30 ZEU/0260

Beyond electrostatic screening: Effect of ion pairing on acid-base equilibria in complex electrolyte solutions — •Varun Mandalaparthy[1], Johannes Hunger[2], Mischa Bonn[2], and Nico van der Vegt[1] — [1]Technical University, Darmstadt — [2]Max Planck Institute for Polymer Research, Mainz

The modulation of acid-base equilibria by salts is central to solution chemistry, yet the molecular origins of these effects in multi-component electrolyte mixtures remain incompletely understood. Building on evidence that individual salts induce ion-specific shifts in the pKa values of weak acids, we combine experiments with constant-pH molecular dynamics simulations to examine how ion pairing and specific ion interactions regulate the pKa of acetic acid in single and mixed sodium salt solutions. Across anions of differing charge density (sulfate, chloride, iodide), we show that cation-anion association-rather than electrostatic screening alone-governs the observed pKa changes. In solutions containing mixtures of sodium chloride and sodium sulfate, the impact on acetic acid pKa deviates from simple additivity because of complex ion-ion interactions. We present an ion-pairing-enhanced Debye-Hückel model that quantitatively reproduces these behaviors, offering a predictive framework for pH regulation in multi-salt environments. This work provides a mechanistic foundation for interpreting and forecasting pH-dependent behavior in complex systems relevant to biochemistry and soft matter.

REF: Mandalaparthy et al. ChemRxiv. 2025; doi:10.26434/chemrxiv-2025-p2chl (under review at J. Phys. Chem. Lett.)

CPP 13.3 Mon 15:45 ZEU/0260

How polymer chain flexibility influences orientation and entanglements in polyelectrolyte solutions — Sascha Bartosch and •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V.

Entanglements in long-chain polymers are important for their mechanical properties and strongly impact the processability. In solutions the formation of entanglements depends on chain length, concentration and the chain flexibility. The flexibility of polyelectrolyte chains is influenced by the ionic strength of the solution that may screen the repulsive electrostatic interaction along the chain. That is reflected in the variation of the hydrodynamic radius of the polyelectrolytes measured by diffusion NMR. Upon shear polymers can orient or polymer chains maybe pulled out of entanglements. The NMR transverse relaxation time T2 is a good measure for the slow polymer-chain dynamics affected by polymer entanglements. Aligning polymer chains results in a shortened T2 while the loss of entanglements yielding longer chain segments between entanglements results in a longer T2. Short-chain polyelectrolytes under shear in a Searle cell show chain orientation. Long-chain polyelectrolytes at low ionic strength orient as well, while at higher ionic strength a loss of entanglements is observed. The transition from stiff to flexible entangled polymer is triggered solely by the electrostatic interaction modulated by the ionic strength under experimental control.

CPP 13.4 Mon 16:00 ZEU/0260

Molecular Mechanisms Underlying LCST and UCST Transitions in Thermoresponsive Ionic Liquids — •Hussen Oumer Mohammed[1,2], Abel De Cozar[1,2], and Ronen Zangi[1,2] — [1]Donostia International Physics Center (DIPC), Donostia, Spain — [2]University of the Basque Country UPV/EHU, Donostia, Spain

We investigate liquid-liquid phase separation (LLPS) of ionic liquid (IL)-water mixtures through atomistic MD simulations. Two model systems are studied: [P_{4444}] [TMBS], which exhibits a lower critical solution temperature (LCST) phase separation, and [Hbet][Tf_2N], which displays an upper critical solution temperature (UCST) behavior.

Aiming to elucidate the driving forces governing the two types of phase separation, we performed a detailed analysis of energy decompositions, HB networks, and microstructural organizations. We find that for [P_{4444}][TMBS]/water phase demixing, increasing temperature weakens IL-water HB, augments the enthalpic penalty of hydration, and favors ion pairing and mesoscale segregation. Conversely, for [Hbet][Tf_2N]/water demixing, cooling enhances water self-networking and suppresses ion hydration, promoting like-like association, while heating disrupts the water network and re-establishes miscibility through stronger ion-water HB.

By shedding light on these molecular-level mechanisms underlying those behaviors in distinct ILs, this study offers a predictive simulation-based framework for the rational design of thermoresponsive draw solutes in FO desalination, enabling tunable and energy-efficient regeneration cycles.

CPP 13.5 Mon 16:15 ZEU/0260

Machine-Learning Prediction of Ionic Conductivity from Short-Time Structural Data in Ionic Liquids — •David Bienek — Helmholtz-Institut Münster, Münster, Germany

Molecular dynamics (MD) simulations are a powerful tool for studying electrolyte materials, but the reliable calculation of ionic conductivities and transference numbers requires long trajectories. In this project, we explore whether machine-learning (ML) models can predict dynamic properties of ionic liquids (ILs) from structural information obtained in much shorter simulations. ILs are chosen as model systems because prior work has demonstrated links between structure and hydrodynamic behaviour. Their simple cation-anion composition also allows systematic generation of simulated systems. As structural descriptors, we employ radial distribution functions (RDFs), which are physically interpretable.

We test linear regression, random forests, and neural networks for predicting ionic conductivity. After feature engineering we find substantial improvements in accuracy. A peak-based representation proves particularly helpful for identifying structure-dynamics relations. Feature-importance analyses consistently indicate that the dominant information originates from the first coordination shell. Moreover, simpler models (random forest, linear regression) outperform neural networks, highlighting the necessity to use appropriate model complexity. Overall, our results show that ML can support the identification of structure-dynamics correlations in electrolytes and may help estimate transport properties from short MD trajectories.

CPP 13.6 Mon 16:30 ZEU/0260

Dissociation of weak polyacid systems in solution and brush coatings determined by IR titration — •Martin Müller[1,2], Luise Wirth[1,2], Birgit Urban[1], Leo Dagand[1,2], Alexander Münch[1], and Petra Uhlmann[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, Dresden D-01069, Germany — [2]Technische Universität Dresden, Dresden D-01062, Germany

The dissociation degrees a of poly(acrylic acid) (PAA) and propionic acid (PA) solutions were determined by infrared (IR) titration and potentiometric (POT) titration concept. Stepwise increasing pH value from 2 to 12 by adding NaOH portions, IR spectra of PAA and PA show decrease of n(C=O) band due to carboxyl (COOH) and increase of n(COO-) band due to carboxylate (COO-) groups. From the respective normalized band integrals A, dissociation degree was calculated according to a=A(COO-)/(A(COOH)+A(COO-)). Plotting pH versus a and fitting by modified Henderson-Hasselbalch equation according to pH=pKa+B*log(a/(1-a)) the parameters pKa and B were determined. The slight pKa deviation found for IR and POT titration, the respective deviation between monomeric PA and polymeric PAA and the PAA molecular weight trend (PAA-2K, PAA-50K, PAA-450K) are discussed considering the two-phase model of polyelectrolyte solutions and Gibbs-Donnan theory. Furthermore, a and pKa of thin PAA brush coatings under aqueous ambient and the influence of metal ion type (Na+, Ca++, Ce+++) and concentration were determined by FTIR titration revealing higher pKa values compared to solution state and significant effects of ion valency on a.

CPP 13.7 Mon 16:45 ZEU/0260

Unconventional Layer-by-Layer Assembly of Films with PEDOT: Write, Read, and Delete — •Muhammad Khurram, Martin Hunger, and Christiane A. Helm — muhammad.khurram@uni-greifswald.de

PEDOT:PSS films are widely used because they offer high conductivity & tunable electro-optical properties. We present an unconventional layer-by-layer (U-LbL) method for PEDOT:PSS/PDADMA multilayers. Masking was used to create either homogeneous coatings or narrow conductive strips. Each bilayer is only 7-9 nm thick, indicating that films form by adsorption of PSS-linked PEDOT, with unbound nanoparticles removed during rinsing. Flow-cell produces higher conductive films (260 kS/m) than dip coating. The U-LbL process also provides a natural framework for repeated Write/Read/Delete modulation, including PEDOT addition, partial & controlled PEDOT removal, forming molecular cavities that rebind PEDOT & restore percolative pathways.

CPP 14: French-German Session: Simulation Methods and Modeling of Soft Matter II

Time: Monday 17:15–19:00 Location: ZEU/LICH

CPP 14.1 Mon 17:15 ZEU/LICH

Lateral interactions in Bisphenol A adsorption on Carbon Nanotubes — •Oliver Cunningham and David Wilkins — Queen's University Belfast, Belfast, Northern Ireland

Endocrine disrupting chemicals (EDCs) such as Bisphenol A (BPA) are being found in water supplies with increasing frequency and our methods of water treatment need to improve alongside this ever increasing problem to mitigate the risks they pose to human health. Molecular Dynamics paired with enhanced sampling methods such as Metadynamics have proven to be very effective at studying the free energy profiles for processes like adsorption. To this end we present the effects lateral interactions between BPA molecules have on their adsorption onto a single walled carbon nanotube (SW-CNT) and how this depends on the number of BPA. The free energy of adsorption is studied as it gives insight into how well a SW-CNT adsorbs BPA and therefore how effective it is at removing it from water. Studying the free energy of adsorption for systems with varying numbers of BPA, we find that the free energy of adsorption increases with the number of BPA. This shows that lateral interactions between BPA molecules have a noticeable effect on how well they adsorb on the surface. We find two free energy minima corresponding to different conformations of the BPA, and the energy barrier between these minima decreases with the number of BPA. We also show that Parallel Bias Metadynamics provides an efficient way to bias all of the BPA in a system, providing better statistics than individually biased runs, while still achieving free energy's adsorption in agreement with the individual runs.

CPP 14.2 Mon 17:30 ZEU/LICH

Multiscale Modeling of Grain Boundary Effects on Charge Transport in Pentacene — •Sonali Garg, Farhad Ghalami, and Marcus Elstner — Karlsruhe Institute of Technology, Karlsruhe, 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 structural defects that affect charge-carrier movement and reduce mobility. In this study, we developed a model to investigate the influence of GB characteristics, including misorientation angles and GB width, on charge carrier mobility, and compare the results with intrinsic mobility. Non-Adiabatic Molecular Dynamics (NAMD) simulations, employing the 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 GBs 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 14.3 Mon 17:45 ZEU/LICH

A classical model to describe the electric potential-dependent water structure at metal interfaces — •Damien Toquer[1], Henrik Stooss[1], Philipp Stärk[1,2,3], and Alexander Schlaich[1] — [1]Institute for Physics of Functional Materials, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Institute for Computational Physics, University of Stuttgart, 70569 Stuttgart, Germany — [3]SC Simtech, University of Stuttgart, 70569 Stuttgart, Germany

Nano- and microfabrication enable the development of functional materials tunable across length scales. While atomistic simulations are a powerful tool for studying and designing such materials bridging atomic-to-macroscopic properties remains challenging. The electrode/water interface exemplifies this challenge, explicit electronic treatment limits simulation scalability. Various schemes have been proposed that aim to incorporate metallic electronic response into classical molecular dynamics. Recently, the constant potential method has shown promise, where charges are attached to the metal atoms to maintain a fixed electrode potential. Our goal is to develop an efficient classical model that reproduces interfacial water structure across various electrode potentials, using gold surfaces as a prototype. Gold charges are adjusted to capture long-range continuum electrostatic interactions, while short-range interactions are tuned to match ab initio energy calculations. We anticipate this model will reliably predict interface-dependent thermodynamic properties both at equilibrium and under applied electrode potential, and plan to use it to study electrowetting in parallel with experimental work.

CPP 14.4 Mon 18:00 ZEU/LICH

Acoustic Effects in Electrolytes with Interfaces: Mechanistic Insights from MD Simulations — •Katharina Kintrup[1], Youssef Mabrouk[1,2], Diddo Diddens[1,3], and Andreas Heuer[1] — [1]Universität Münster, Institut für Physikalische Chemie, Deutschland — [2]Friedrich-Schiller-Universität Jena, Institut für Physikalische Chemie, Deutschland — [3]Helmholtz-Institut Münster, Deutschland

Interfaces such as electrodes strongly affect transport and dynamics in electrolytes. However, Molecular Dynamics (MD) simulations often assume periodic boundary conditions (pbc), thereby neglecting interfacial effects. This enforces a fixed center-of-mass frame in simulations, whereas electrophoretic NMR (eNMR) experiments [1,2] have shown that, in laboratory electrolytes, the center of mass drifts and local volume conservation is the appropriate assumption.

To mimic laboratory conditions, we introduce explicit interfaces in MD simulations and employ external fields for comparison with eNMR. As expected, we also observe a drift of the center of mass, but we do not find ideal local-volume conservation. Instead, we obtain oscillatory signals that reveal a strong dominance of acoustic effects over the intrinsic ionic dynamics. For binary electrolytes, we formulate a theoretical description that accurately incorporates the finite compressibility of the fluid. Overall, our work provides spatial and temporal insights into electrolyte dynamics in the presence of interfaces and highlights the importance of the chosen reference frame. [1] J. Phys. Chem. Lett. 2022, 13, 37, 8761-8767; [2] ACS Appl. Polym. Mater. 2025, 7, 13, 8432-8444

CPP 14.5 Mon 18:15 ZEU/LICH

Understanding electrode/electrolyte interfaces for electrocatalysis using constant potential DFT simulations — •Henrik Stooss[1], Philipp Stärk[2], and Alexander Schlaich[1] — [1]Institute for Physics of Functional Materials, Hamburg University of Technology, 21071 Hamburg — [2]Institute for Computational Physics, Universität Stuttgart, 70569 Stuttgart

This study explores the complex dynamics at electrode/electrolyte interfaces under constant potential, which is crucial for advancing electrocatalysis and designing efficient energy systems. We combine advanced computational techniques to gain insights into the mechanisms at these interfaces. Specifically, we perform Density Functional Theory (DFT) simulations of interfacial systems while maintaining a constant electrode potential. Despite the associated challenges and computational costs, these simulations provide valuable insights into the electronic structure and behavior of electrode surfaces. We calculate IR spectra of water in front of a gold electrode at different applied potentials and compare the results with experimental ATR-SEIRAS data, thereby strengthening the connection between first-principles calculations and experimental observations for material design.

CPP 14.6 Mon 18:30 ZEU/LICH

Atomistic modeling of azopolymers: light-induced deformation — •Dmitry Ryndyk[1,2], Olga Guskova[1], and Marina Saphiannikova[1,2] — [1]Leibnitz Institute of Polymer Research Dresden, Germany — [2]Technische Universität Dresden, Germany

In our recent study [1], we employ, for the first time, a fully atomistic force-field approach to model light-induced deformations in side-chain azopolymers. To mimic sample illumination, we introduce an orientation potential that reorients the azo chromophores perpendicular to the light polarization direction. This strategy enables us to capture both the microscopic details of chromophore behavior and the collective, anisotropic response of the polymer matrix. The atomistic simulations show a clear correlation between chromophore reorientation and sample contraction, as well as between backbone alignment and sample elongation. The separation of time scales between these two processes is controlled by the relative distance to the glass-transition temperature. Furthermore, the simulations elucidate a role of the flexible spacer in transferring the light-induced torque to the polymer backbone.

[1] D.A. Ryndyk, O. Guskova, M. Saphiannikova, Light-induced deformation of side-chain azo-polymer: Insights from atomistic modeling, arXiv:2511.19787 (2025)

CPP 14.7 Mon 18:45 ZEU/LICH

Self-Assembly of Porphyrin-Based Monomers into Supramolecular Polymers — •Mira Mors[1], Hanna Rieger[2], Oliver Stach[2], Thomas Speck[1], and Pol Besenius[2] — [1]Institute for Theoretical Physics IV, University of Stuttgart, Germany — [2]Department of Chemistry, Johannes Gutenberg-University Mainz, Germany

Through a combination of computational modeling and experiments, we investigate the assembly pathways of water-soluble supramolecular porphyrin-peptide amphiphiles. Our computational approach employs a coarse-grained, nine-bead planar model that captures the essential molecular interactions. Simulations show that stronger interactions promote polymerization, whereas increased monomer flexibility hinders it, consistent with experiments in which an additional glycine is introduced into the peptide arms. The observed power-law dependence of the polymerization half-time suggests a nucleation-elongation-aggregation pathway; however, experiments show no concentration-dependent aggregation. To probe oligomer stability, we apply a simplified free energy model and enhance sampling by generating a grand canonical system to map free energies across cluster sizes. Aggregation kinetics are additionally studied by solving the rate equations explicitly and using moment-based approaches. These analyses reproduce the dynamics from low to high interaction strengths, highlighting the vital role of recombination in the polymerization regime. Overall, our results provide a framework for a better understanding of supramolecular polymerization under varying conditions.

CPP 15: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods II

Time: Monday 17:15–19:00 Location: ZEU/0255

CPP 15.1 Mon 17:15 ZEU/0255

Deep Learning-Driven Grazing Incidence Small-Angle X-ray Scattering Data Processing for Nanostructure Characterization — •Yufeng Zhai[1], Jungui Zhou[1], Shachar Dan[1], Julian Heger[2], Benedikt Sochor[1,3], Arno Jeromin[4], Wenbo Wang[5], Wolfgang Parak[5], Sarathlal Koyiloth Vayalil[1,6], Thomas Keller[4,5], Andreas Sitierle[4,5], Alexander Hexemer[3], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,7] — [1]DESY, Hamburg, Germany — [2]TUM, Garching, Germany — [3]ALS/LBNL, California, United States — [4]CXNS, Hamburg, Germany — [5]UHH, Hamburg, Germany — [6]UPES, Dehradun, India — [7]KTH Stockholm, Sweden

Nanostructured thin films formed via nanoparticle deposition or self-assembly exhibit diverse morphologies that are crucial for their functional properties. Grazing-incidence small-angle X-ray scattering (GISAXS) provides detailed structural information on such systems, but conventional model-based fitting remains limited by simplified assumptions and convergence difficulties. We employ the distorted wave Born approximation (DWBA) to simulate a wide range of two-dimensional GISAXS patterns, which are used to train convolutional neural networks (CNNs) for predicting nanoparticle size distributions. The trained models demonstrate robust performance on both simulated and experimental data, providing a faster and more flexible alternative to traditional fitting. In addition, we have developed a graphical user interface (GUI) that integrates conventional fitting routines with our deep learning framework, providing a user-friendly platform for rapid GISAXS analysis.

CPP 15.2 Mon 17:30 ZEU/0255

Chirp-DMA for expanded frequency and reduced aging — •Juan Pablo Segovia Gutiérrez[1], José Alberto Rodríguez Agudo[2], Jan Haeberle[2], Dominic Oppen[2], Jörg Läuger[2], and Natalie Germann[1] — [1]University of Stuttgart, Stuttgart, Germany — [2]Anton Paar Germany GmbH, Ostfildern, Germany

Optimal Fourier Rheometry (OFR), or Chirp rheometry, is an advanced technique that uses a continuous, sine wave-shaped stress/strain signal characterized by an exponential frequency increase. This approach is important for measuring rapidly time-evolving soft materials, where conventional frequency sweeps are impractical; their slow, sequential data acquisition often fails to capture fast structural changes before the material itself mutates. A key advantage of Chirp is its ability to drastically reduce measurement time, making it highly effective at low and very low frequencies. This speed is essential to circumvent undesirable material aging, for instance in the dehydration observed in hydrogels, which modifies properties during long acquisition times. Conventionally, Chirp has been implemented using standard plate-plate geometries. The novelty of this study is the implementation of Chirp within a Dynamic Mechanical Analysis (DMA) setup utilizing extension and torsion modes. This permits the characterization of soft, fragile materials outside the typical rheometer configuration. By combining this novel Chirp-DMA approach with conventional sweeps on gellan gum/alginate hydrogels, we extend the practical frequency range and prove that Chirp recovers true viscoelastic moduli, thereby eliminating dehydration-induced effects.

CPP 15.3 Mon 17:45 ZEU/0255

PIERS-Based Mechanistic Insights into PVC Micro- and Nanoplastics Degradation on Ag Nanoflake-TiO2 Platform — •Olugbenga Ayeni[1], Josiah Ngenev Shondo[2], Tim Tjardts[3], Sinan Şen[4], Franz Faupel[3], Salih Veziroglu[3], Oral Cenk Aktas[3,4], and Tayebeh Ameri[1] — [1]Chair for Composite Materials, Department of Materials Science, Kiel University, Germany. — [2]Department of Energy Conversion and Storage, Technical University of Denmark, Denmark. — [3]Chair for Multicomponent Materials, Department of Materials Science, Kiel University, Germany. — [4]Department of Orthodontics, University Hospital of Schleswig-Holstein (UKSH), Kiel, Germany.

Conventional characterization techniques such as FTIR and SERS have been applied to Polyvinyl chloride (PVC) micro- and nanoplastics (MNPs) degradation, but they lack the combined real-time sensitivity and photocatalytic functionality needed to probe early-stage PVC-MNPs degradation. In this work, we report the use of Photo-induced enhanced Raman spectroscopy (PIERS) technique under continuous UV illumination to monitor the degradation of PVC-MNPs in real time on a highly active photocatalytic platform based on Ag nanoflakes (Ag NFs) grown on TiO2 thin films. Our PIERS-based approach reveals the chemical transformations and structural disorder occurring in the PVC-MNPs backbone within 10 min of UV irradiation. Our results establish PIERS as a promising mechanistic probe for tracking real-time PVC degradation pathways at the nanoscale. This study advances the mechanistic understanding of plastic degradation at the nanoscale.

CPP 15.4 Mon 18:00 ZEU/0255

Exploring Colloidal Kinetics Using DLS — •Mohit Agarwal and Jiaxing Sun — Swabian Instruments GmbH, Stuttgart, Germany

The kinetic behavior of colloidal and soft matter systems arises from particle diffusion, aggregation, and structural rearrangement, which collectively determine how microstructures evolve over time. Accurate characterization of these dynamics is crucial for understanding nonequilibrium phenomena such as gelation, crystallization, and phase separation in complex fluids. Conventional experimental techniques often lack the temporal and angular resolution needed to resolve these fast and heterogeneous processes in their native state, especially when multiple relaxation mechanisms coexist. We present a time-resolved, multi-angle Dynamic Light Scattering (DLS) technique that records individual photon arrival events in real-time across multiple scattering angles. This configuration enables angle-dependent temporal correlation analysis with improved sensitivity to both short-time diffusive motions and long-time relaxation processes that reflect evolving particle interactions. By employing complete photon statistics rather than time-averaged intensity correlations, the method captures transient fluctuations and kinetic transitions in colloidal suspensions. Measurements on well-defined colloidal dispersions reveal subtle temporal variations in particle dynamics and aggregation behavior that remain inaccessible with conventional single- or multi-angle goniometer-based DLS. The technique establishes a robust framework for real-time, multi-scale investigation of kinetic processes in colloidal and soft matter systems.

CPP 15.5 Mon 18:15 ZEU/0255

The Power of One Oxygen: How a Single Atom Alters the Field Evaporation of Liquid Crystals — •Kuan Meng, Sebastian Eich, and Guido Schmitz — University of Stuttgart, Institute for Materials Science, Heisenbergstr. 3, 70569 Stuttgart, Germany

In this study, we established a cryo-atom probe tomography (cryo-APT) workflow to investigate how the presence of a single oxygen atom alters the field evaporation behavior of two structurally similar liquid crystals: 8CB and 8OCB. Both compounds exhibited over 70% intact molecular retention and comparable fragmentation patterns.

Mass spectra revealed that the oxygen in 8OCB hinders the formation of extended cyanobiphenyl fragments across the linkage and promotes full cleavage of the alkyl chain. In contrast, 8CB allows the formation of longer backbone fragments. Spatially, 8CB evaporated mainly as intact molecules across both crystalline and smectic domains. 8OCB, however, evaporated predominantly as small fragments in low volume-density domains while as larger fragments or intact molecules in the high volume-density regions, which are suspected to crystalline and smectic phases, respectively. Further structural validation is required.

This work illustrates how cryo-APT enables the characterization of the molecular structure of organic liquid systems and demonstrates that even a single oxygen atom can fundamentally alter their field evaporation pathways. It further proposes a tunable fragmentation strategy to investigate molecular orientation in soft matter at an unprecedented resolution.

CPP 15.6 Mon 18:30 ZEU/0255

Depth-resolved cathodoluminescence for mapping exciton diffusion in rubrene thin film polymorphs — •Heiner Thiersch[1,2], Jonas Schröder[1], Anna-Lena Hofmann[1], Wooik Jang[1], Nora Engelmann[1], Fritz Henke[1], Maximilian F. X. Dorfner[3], Shu-Jen Wang[4], Frank Ortmann[3], Johannes Benduhn[1,2], Ellen Hieckmann[1], and Karl Leo[1] — [1]IAPP, TU Dresden, Germany — [2]DZA Görlitz, Germany — [3]Dep. of. Chem., TU München, Germany — [4]Dep. of. Phys., HKBU, China

The exciton diffusion length (L_D) is a key parameter in opto-electronic devices, as it governs the transport and recombination of photogenerated excitons. However, accurately measuring L_D remains challenging due to the limited penetration depth and lateral resolution of conventional techniques such as photoluminescence quenching and transient absorption spectroscopy. Here, we will introduce a novel approach for L_D determination based on quenching processes observed by depth-resolved cathodoluminescence (CL) measurements with highly localized excitation. The method combines CL experiments with kinetic Monte Carlo simulations and a diffusion model derived from Fick's second law. Applied to the organic semiconductor rubrene-renowned for its high hole mobility in single crystals- the technique yields L_D values ranging from 50 to 100 nm across different thin-film polymorphs. The results provide new insights into the exciton dynamics of rubrene and present a new methodological tool for accurate L_D characterization in semiconductors.

CPP 15.7 Mon 18:45 ZEU/0255

Towards Theoretical UV/Vis Spectra with Experimental Accuracy - Functional Errors and Thermal Broadening — •Robert Strothmann[1], Johannes T. Margraf[2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]University of Bayreuth, Bayreuth, Germany

First principles methods like time-dependent density-functional theory (TD-DFT) can be used to predict molecular UV/Vis spectra relying on a number of approximations such as the choice of functionals, the description of solvation, as well as the treatment of thermal broadening. For the latter, simple (smeared) line spectra or structural ensembles obtained within the harmonic approximation are the most common choices. With the rise of machine learning interatomic potentials (MLIP) prohibitively costly *ab initio* molecular dynamics (MD) simulations can be replaced with similarly accurate MLIP MDs. This allows a detailed comparison of these approaches for a large number of systems for the first time.

In this talk, we benchmark predicted UV/Vis spectra against experimental references. To this end, the agreement with a curated set of literature reported spectra for diverse organic molecules in various solvents is assessed in terms of full spectral overlap, beyond a "peak to peak" comparison. We emphasize the influence of functional choice and thermal sampling approaches (e.g. harmonic vs. anharmonic), as well as the role of different conformers. How important each of these effects is and how it affects computational cost will be studied with the goal of providing best practise guidelines.

CPP 16: Energy Storage Materials and Devices II

Time: Monday 17:15–19:00 Location: ZEU/0260

Invited Talk CPP 16.1 Mon 17:15 ZEU/0260

Understanding the Passivation Properties of Solid Electrolyte Interphases (SEIs) in Batteries: Generator-Collector Experiments combined with a Transport and Reaction Model — •Bernhard Roling, Falk Krauss, Annalena Duncker, and Isabel Pantenburg — Department of Chemistry, University of Marburg, Germany

The solid electrolyte interphase (SEI) is a passivation layer in lithium-ion batteries, which has a strong impact on the battery lifetime. The SEI is formed by reductive decomposition of the electrolyte at the graphite particles of the anode during the first charging of the battery. The passivation of the SEI is not perfect, which leads to battery aging and to a reduced battery lifetime. The transport and reaction mechanism in the SEI governing the passivation properties are not well understood. Here, we elucidate transport and reaction processes during the formation of model-type SEIs by combining generator-collector experiments with a transport and reaction model. In the generator-collector experiments, we use a four-electrode-based setup to compare the electrolyte reduction current with a redox molecule reduction current at the SEI-covered electrode. We find that the current ratio depends on the SEI formation potential as well as on the formation time. The experimental results are compared to a transport and reaction model predicting four distinct transport and reaction regimes depending on the rate constant for the molecule-electron reaction. Using this combined approach, we obtain good estimates for the transport coefficients of both electrons and molecules inside the SEI.

CPP 16.2 Mon 17:45 ZEU/0260

Insight into SEI formation and dendrite growth in all-solid-state lithium metal batteries by Operando nWAXS — •Yingying Yan[1], Liangzhen Liu[2], Yuxin Liang[1], Lyuyang Cheng[1], Fabian A.C. Apfelbeck[1], Guangjiu Pan[1], Anton Davydok[3], Christina Krywka[3], Roland A. Fischer[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]TUM School of Natural Sciences, Chair of Inorganic and Metal-Organic Chemistry, Garching, Germany — [3]Helmholtz-Zentrum Hereon, Max-Planck-Str. 1, Geesthacht, Germany

Composite solid polymer electrolytes (CSPEs) have emerged as promising candidates for next-generation all-solid-state lithium batteries (ASSLBs). However, the limited ionic conductivity and poor interphase stability have seriously hindered their practical application. Herein, the anion-trapping layered double hydroxide (LDH) was introduced to enhance ionic conductivity and interfacial compatibility in poly(ethylene oxide) (PEO)-based CSPEs for stabilizing lithium metal anodes. Importantly, operando nano-focus Wide-angle X-ray scattering (nWAXS) was employed to spatially map the distribution of both the solid electrolyte interphase (SEI) layer and lithium dendrites across micron-scale lateral and vertical dimensions. Therefore, this study provides a novel strategy for designing high-performance CSPEs with stabilized interfaces and establishes an innovative approach for real-time visualization of SEI evaluation and dendrite growth in ASSLBs.

CPP 16.3 Mon 18:00 ZEU/0260

Temperature effects on the electrochemical behavior of graphite cathodes for aluminium-polymer batteries — •Mohammad Mostafizar Rahman, Mohammad Jony Rana, Shuvrodev Biswas, Amir Mohammad, Hartmut Stöcker, and Dirk C. Meyer — Institute of Experimental Physics, TU Bergakademie Freiberg, Leipziger Str. 23, Freiberg, 09599, Germany

This study assesses the performance of Aluminium-polymer batteries at variable temperatures between $-20\,^\circ\mathrm{C}$ and $80\,^\circ\mathrm{C}$. Pouch cells were constructed utilizing a solid polymer electrolyte (SPE) coupled with two different types of graphite cathode: mesocarbon microbeads (MCMB) and spherical graphite (SpG). Cyclic voltammetry and galvanostatic cycling with potential limitation measurements were conducted at different temperatures combined with variable current densities (25...100 mA/g). The results reveal that the resistance degradation below $0\,^\circ\mathrm{C}$ is reversible, with performance being recovered when returning to positive temperatures. However, at moderately high temperatures above $60\,^\circ\mathrm{C}$, the degradation becomes permanent. MCMB cells operate effectively between $-10\,^\circ\mathrm{C}$ and $40\,^\circ\mathrm{C}$, while SpG cells function from $0\,^\circ\mathrm{C}$ to $60\,^\circ\mathrm{C}$. The capacity of MCMB cells peaks at $20\,^\circ\mathrm{C}$ at all current densities and then drops significantly at $60\,^\circ\mathrm{C}$. In contrast, SpG cells exhibit their highest capacities at $40\,^\circ\mathrm{C}$ or $60\,^\circ\mathrm{C}$, followed by a rapid decline. Together with the good Coulombic efficiencies $> 95\,\%$ both types of cells are proven suitable for varying environmental conditions.

CPP 16.4 Mon 18:15 ZEU/0260

X-Ray Absorption Near-Edge and Photoemission Spectroscopy of Deintercalation and Redox Reactions in Alluaudite-Type Na-Ion Cathodes — •Neama Imam[1], Karsten Henkel[1], Stephan Werner[2], Christoph Pratsch[2], Anna Milewska[3], Janina Molenda[3], Jan Ingo Flege[1], and Ehrenfried Zschech[1] — [1]Brandenburg University of Technology Cottbus - Senftenberg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY II, Germany — [3]AGH University of Science and Technology, Krakow, Poland

We have investigated alluaudite-type $\mathrm{Na_{2.5-\mathit{x}}Fe_{1.75}(SO_4)_3}$ cathodes that exhibit a three-dimensional open-channel framework with multiple Na sites. Using spatially resolved X-ray absorption near-edge spectroscopy (XANES), performed within a transmission X-ray microscope (TXM), and lab-based X-ray photoelectron spectroscopy (XPS), we have examined $\mathrm{Na^+}$ deintercalation and $\mathrm{Fe^{2+}/Fe^{3+}}$ charge compensation at different selected charging states. This combination of bulk- and surface-sensitive methods allows correlating Na^+ depletion with Fe^{3+} formation, potentially identifying nanoscale redox heterogeneities and tracking changes in the local Na chemical environment. Our study builds on a broader investigation [1] that includes theoretical calculations as well as structural and electrochemical analyses.

[1] J. Molenda *et al.*, *Acta Mater.* **301**, 121582 (2025).

CPP 16.5 Mon 18:30 ZEU/0260

Understanding the Impedance Spectra 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, Germany — [2]Center for Materials Research (ZfM), Justus-Liebig-University Giessen, Germany — [3]Institute of Physical Chemistry, Justus-Liebig-University Giessen, Germany

All-solid-state batteries (ASSBs) are promising candidates for next-generation energy storage systems, offering enhanced energy density and safety compared to conventional lithium-ion batteries. Electrochemical Impedance Spectroscopy (EIS) is a powerful method for determining charge transport characteristics in these systems. However, the presence of multiple phases, each with distinct transport processes, as well as complex microstructures result in complex impedance spectra that are challenging to interpret.

To address this challenge, we use a microstructure-resolved 3D electrical network model to simulate charge transport on microscopic length scales. This approach enables us to disentangle the contributions of different transport processes and microstructural features to the impedance response. Our model offers insights into the local potential and current distributions influenced by material heterogeneities, directly connecting them to impedance signals. We provide insights into the impedance of composite materials, identifying the key factors that dominate the impedance signal.

CPP 16.6 Mon 18:45 ZEU/0260

Dual-Ion $AlCl_4^-$ / $AlCl_2^+$ Charge Storage Mechanism in Composite Cathode for Aluminum-Polymer Batteries — •Shuvrodev Biswas, Thomas Köhler, Amir Mohammad, Hartmut Stöcker, and Dirk C. Meyer — Institute of Experimental Physics, TU Bergakademie Freiberg, Leipziger Str. 23 09599 Freiberg, Germany

Rechargeable aluminum batteries have emerged as a promising post-lithium-ion technology. Graphite, the most widely used cathode that relies on $AlCl_4^-$ intercalation, offers limited capacity, whereas organic cathodes, such as phenanthrenequinone (PQ), coordinate with $AlCl_2^+$ but suffer from limited cycling stability. Here, we design a composite (SPGPQ) consisting of spherical graphite (SPG) and PQ through melt diffusion, enabling dual-ion charge storage by coupling $AlCl_4^-$ intercalation with $AlCl_2^+$ coordination. FTIR, XPS, *in situ* XRD, and cyclic voltammetry using polyamide-6 (PA6) electrolytes (SPE) provide clear evidence of this synergistic mechanism. Whereas the PA6-SPE limits capacity due to low ionic conductivity, the higher-conductivity polyacrylonitrile (PAN)-based SPE delivers improved capacity but shows limited cycling stability. To enhance stability, we further developed an ACPQ+SPG composite through solvent-assisted impregnation using activated carbon (AC). This composite features an identical mechanism to SPGPQ, while offering significantly enhanced capacity and stable long-term cycling.

CPP 17: Poster I

Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates; Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics; Energy Storage Materials and Devices; French-German Session: 2D Materials, Thin Films and Interfaces; Wetting, Fluidics and Liquids at Interfaces and Surfaces

Time: Monday 19:00–21:00 Location: P5

CPP 17.1 Mon 19:00 P5

How do interfaces shape molecular conformations in condensates? — •Nora-Elen Giesinger[1] and Arash Nikoubashman[1,2] — [1]Leibnitz-Institut für Polymerforschung, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany

The interface between biomolecular condensates and their surrounding environment plays an important role for, e.g., regulating the condensate's stability and interactions with other cellular components. These interfacial properties are primarily dictated by the density and conformation of the constituent biomolecules, but it remains experientially challenging to resolve interfacial properties on the molecular level. Further, the conformations of the constituent biomolecules are influenced by many intertwined factors like sequence patterning, electrostatics, and chain-length diversity. To understand how polymer conformations evolve from the dense condensate interior through the interfacial region into the surrounding dilute phase, we use a minimal model of fully flexible homopolymers. To disentangle effects arising from chain ends, we examine condensates formed from both linear and ring polymers. Molecular dynamics simulation show that polymers gradually collapse as they transition from the bulk-like interior of the condensate to the surrounding dilute aqueous phase. Notably, the condensate interface induces a highly non-monotonic structural crossover between the dense and dilute regions, irrespective of the polymer architecture: the side facing the interface flattens, while the inward-facing side is also compressed. As a result, the monomer cloud loses its spherical symmetry, and chains tend to align tangentially along the interface.

CPP 17.2 Mon 19:00 P5

Effects of Activity on Polymeric Condensates — •Rahul Yadav[1] and Arash Nikoubashman[1,2] — [1]Leibnitz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01069 Dresden, Germany

Biological systems are inherently out of equilibrium as external sources of energy are constantly consumed; for example, microtubules and filamentous actin seemingly move through the cytoplasmic matrix via the continuous addition and removal of subunits. At the same time, equilibrium thermodynamic properties, governed by the interactions and length scales of the (macro)molecular constituents, play a central role in phenomena such as the formation of biomolecular condensates. A central open question is whether such non-equilibrium activity enhances phase separation or, conversely, hinders it. To answer this, we performed molecular dynamics simulations of a bead-spring polymer model, systematically varying both the attrac- tion strength and activity. When the active forces act along the contour of the polymer, the miscibility gap narrows and the critical temperature decreases with increasing activity, indicat- ing that this form of activity opposes phase separation. Based on these observations, we expect that contractile active forces will instead broaden the miscibility gap and increase the critical temperature, and we plan to test this prediction in future work.

CPP 17.3 Mon 19:00 P5

Using the Patchy Particle Model to simulate Biomolecular Condensates — •Mubarrat Mursalin[1,2], Simon Dannenberg[1], and Stefan Klumpp[1,2] — [1]Georg August University Göttingen — [2]Max Planck School of Matter to Life

Biomolecular condensates are formed through liquid-liquid phase separation (LLPS) of proteins, often together with nucleic acids, typically driven by low-affinity interactions. Phase separation allows biological systems to spatially organize molecules for biological functions. Theoretical studies of LLPS are usually based on continuum descriptions of fluids, which allows access to the biologically relevant time and length scales, but neglects all molecular details of the interactions, which implements their genetic programmability and determines the local structure of the condensates. Here, we use the coarse grained patchy particles to simulate LLPS, which provides an intermediate level of description between atomistic MD and continuum descriptions, thus allowing to access systems large enough to describe droplets and still retain a coarse-grained picture of the local structure inside the condensate. We look at the effects of repulsive crowding particles on the critical values, dynamics and structures of biomolecular condensates formed by three patch patchy particles. Using NVT simulations, combined with the direct coexistance method, we study the effects of crowder concentration and size, and recreate the known depletion and excluded volume effects.

CPP 17.4 Mon 19:00 P5

Partial demixing of RNA Polymerase II condensates in transcription regulation — Arya Changiarath[1], Rosa Herrera Rodriguez[1], Jasper Michels[3], Friederike Schmid[1], Jan Padeken[2], and •Lukas Stelzl[1,2] — [1]Johannes Gutenberg University Mainz — [2]Institute of Molecular Biology (IMB) — [3]Max Planck Insitute for Polymer Research

Phase-separated condensates may spatio-temporally regulate RNA polymerase II (Pol II) during the transcription of genes. Distinct condensates may underpin the two key stages of transcription, initiation and elongation. However, it remains unclear whether these condensates mix or maintain distinct chemical environments. To investigate this, we combined multi-scale molecular dynamics simulations with experiments in C. elegans. We identified a lower critical solution temperature (LCST) behavior for Pol II, where higher temperatures promote condensation. This behavior correlates with an incremental transcriptional response to temperature but is largely uncoupled from the classical heat stress response. Our simulations demonstrate that the phosphorylation state of the disordered CTD controls the demixing of CTD and pCTD, resulting in full or partial engulfment depending on composition. Remarkably, we observe such partially-demixed of RNA polymerase II condensates by super resolution microscopy of C. elegans embryos. Overall, our results suggest that partially demixed condensates provide distinct chemical environments and binding platforms to facilitate transcription initiation and elongation.

CPP 17.5 Mon 19:00 P5

Optimization of Slot-Die Printed Organic Solar Cells — •Dinusha M. Egalla, Christoph G. Lindenmeir, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Organic solar cells (OSCs) are promising candidates for lightweight, flexible, and low-cost photovoltaic technologies due to their solution processability and compatibility with large-area printing. The performance and stability of printed OSCs, however, are highly influenced by the morphology and uniformity of the active layer, which are sensitive to changes in coating and processing conditions. In this work, we investigate the optimization of printed donor-acceptor active layers by systematically varying key fabrication parameters, including coating temperature, printing speed, and solution preparation. The resulting thin films are characterized using UV-Vis spectroscopy to evaluate optical absorption, and microscopy to investigate the film homogeneity, while X-ray reflectivity (XRR) is used to determine film thickness and roughness. Full devices are built and assessed through current-voltage (J-V) measurements under standard illumination to establish how different printing conditions affect active-layer morphology and overall photovoltaic performance.

CPP 17.6 Mon 19:00 P5

Tuning Two-Photon Absorption Cross Sections in Azaacene Diradicals — •Gabriel Sauter[1], Antonia Papapostolou[2], Julia Weyandt[1], Pascal Merten[3], Kerstin Brödner[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

Diradical bithiophene azaacenes have been shown as an outstanding class of nonlinear optical (NLO) materials with potential applications in bioimaging, photodynamic therapy, and 3D nanoprinting, while exhibiting exceptionally high two-photon absorption (2PA) cross sections exceeding 53000 GM [1]. Using a combined approach of experimental z-scan measurements and theoretical modeling, we analyzed the structure-property relationships governing NLO efficiency and tuning. Here especially the influence of diradical character, molecular extension, and sulfur substitution on the 2PA response was investigated. The results reveal fundamental insights into the synergy between molecular symmetry and electronic structure for optimizing the NLO responses. This enables a more targeted design of near-infrared active materials for photonic applications.

[1] G. Sauter, A. Papapostolou et al., *Angew. Chem. Int. Ed.* 2025, 64, e2503073.

CPP 17.7 Mon 19:00 P5

Long Chain, Strong Gain: How SubPC side chains control the pseudoferroelectric bulk photovoltaic effect — •Kaspar Haas[1], Sophia Klubertz[1], Victor Rodriguez[2], David González-Rodríguez[3], Miguel García Iglesias[2], and Martijn Kemerink[1] — [1]Universität Heidelberg, Heidelberg — [2]Universidad de Cantabria, Santander — [3]Universidad Autónoma de Madrid, Madrid

While most studies of the bulk photovoltaic effect (BPE) in recent years have focused on inorganic materials, this fascinating effect should also be observable in organics. In contrast to the conventional photovoltaic effect, the BPE voids the need for doping by utilizing an intrinsic symmetry breaking and could allow for wider absorption spectra while theoretically overcoming the Shockley-Queisser limit. Going organic holds the additional promise of lightweight, low-fabrication- and low-energy-cost devices, and, particularly, of a much greater tunability of the active material.

Here, we investigate organic molecules of the semiconducting π-conjugated SubPC-F family with the purpose of finding and quantifying a bulk photovoltaic effect. Combining electrical measurements with polarization optical microscopy (POM), XRD and AFM, we investigate the dipole alignment in these liquid crystalline materials, before assessing their photovoltaic performance under irradiation. We further build our own liquid crystal cells for measuring in out-of-plane structures to draw a connection between device thickness and performance. We also aim to quantify the influence of different side chain lengths on material properties like open-circuit voltage and photocurrent.

CPP 17.8 Mon 19:00 P5

Thin Films of Substituted Imidazoquinolines as Emitters for Blue OLED Devices — •Lasse Freitag[1], Pascal Schweitzer[1], Carina Rössiger[2], Thomas Oel[2], Richard Göttlich[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 semiconductors are routinely applied in microelectronics. Still challenging is the field of organic blue light emitting diodes (OLED), due to degradation of the emitters. We study the application of imidazoquinolines such as 4EstPhPh(iso)IC as emitters. Different substitutional patterns allow for tuning of their opto-electronic properties. We achieved thin films of 4EstPhPh(iso)IC via physical vapor deposition (PVD). Promising blue photo- and electroluminescence was found in solid state. Film formation at interfaces with contact materials was studied by in-situ Kelvin-probe force microscopy (KPFM). On the p-conducting poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) we found a Stranski-Krastanov (SK) growth of the emitter. X-ray diffraction (GI-XRD) confirmed a crystalline structure in these films, in line with single crystal data. Further, the growth of n-conducting bathocuproine (BCP) on the emitter layer was monitored by KPFM, revealing SK growth followed by formation of 3D crystalline islands. As a fundamental prerequisite, morphological stability at air was confirmed by microscopy. Therefore, we built OLED with varying thickness to find the best-performing layer stack.

CPP 17.9 Mon 19:00 P5

The aggregation of DPND dyes in the solid state studied by nuclear magnetic resonance spectroscopy — •Sascha Bartosch[1], Mohamed Bouajhine[2], Łukasz Kielesiński[3], Marieta Levichkova[4], Eva Bittrich[1], Petra Uhlmann[1], Patrick Brocorens[2], Martin Pfeiffer[4], Daniel T. Gryko[3], David Beljonne[2], and Ulrich Scheler[1] — [1]Leibniz-Institut für Polymerforschung Dresden e. V. - Dresden, Germany — [2]Laboratory for Chemistry of Novel Materials, University of Mons - Mons, Belgium — [3]The Institute of Organic Chemistry of the Polish Academy of Sciences - Warsaw, Poland — [4]Heliatek GmbH - Dresden, Germany

Dipyrrolonaphthyridinediones (DNPDs) have recently been introduced as a novel class of cross-conjugated dyes. Their promising photophysical properties make them a potential candidate for various applications. Although the packing type is expected to have an influence on the performance, their aggregation remains to be studied.

Solid-state NMR 1H-1H double-quantum-single-quantum correlation experiments are suitable to probe the spatial proximity of functional groups since it is based on short-range dipolar interactions between the spins. The proximity information is used for the understanding of the packing of molecules. Signals have been assigned by comparison of the experimental to simulated chemical shifts. Strong up-field shifts of aromatic protons induced by packing effects like pi-pi-interactions were observed, consistent with predicted crystal structures. Intermolecular homo couplings were used to identify different aggregation patterns.

CPP 17.10 Mon 19:00 P5

Influence of antisolvents and interfacial layers on charge carrier dynamics of hybrid perovskite films — •Leon Weintz[1], Patrick Dörflinger[1], Volodymyr Vasylkovskyi[1], Junmo Park[2], Hobeom Kim[2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany — [2]Department of Materials Science and Engineering, Gwangju Institute of Science and Technology, 61005, Gwang-ju, Republic of Korea

Charge carrier behavior in perovskite thin films is crucial to their optoelectronic performance; yet, the impact of antisolvents and self-assembled monolayers (SAMs) on their basic charge carrier transport properties remains not fully understood. In this work, FAPbI$_3$ and FAMACsPbBr$_3$ perovskite systems are investigated to gain a more comprehensive understanding of how processing additives influence charge generation, transport, and recombination. The mobility and lifetime of photogenerated charge carriers in perovskite layers are determined in a non-contact way using Time-Resolved Microwave conductivity (TRMC), where the interaction of an applied electro-magnetic field with the charge carriers results in a time-dependent change in conductance. Complementary time-resolved photoluminescence (trPL) measurements support the interpretation of TRMC-derived carrier dynamics. Together, TRMC and trPL provide insight into how processing additives influence charge-carrier dynamics in perovskite materials.

CPP 17.11 Mon 19:00 P5

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

We investigate the excited state dynamics of conjugated thiophen based polymers using several kinetic models commonly discussed in the literature. These models describe scenarios in which a short lived excited state acts as a precursor for one or more long lived states and are formulated through coupled rate equations. Four representative models were fitted to the dynamics of DPP4T-1 and subsequently applied to pDPP4T, DPP DTT, pF8T2 and pTDPP to identify trends linked to structural variations within the polymer series. This analysis provides a coherent framework for comparing relaxation pathways and for assessing how precursor states influence the formation of long lived excited state populations.

CPP 17.12 Mon 19:00 P5

Tuning the switching response of purely organic photonic devices by polymer blending — •Jinghan Lin, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden, Dresden, Germany

Programmable luminescent tags (PLTs) provide a promising photonic technology for UV sensing by utilizing the oxygen-sensitivity of room-temperature phosphorescence (RTP) from purely organic emitters [1]. In the emissive layer, the emitter molecules are diluted at low concentration in a rigid polymer host, like Polystyrene (PS) or Poly(methyl methacrylate (PMMA), to reduce photonic loss mechanisms, e.g. triplet-triplet annihilation and non-radiative relaxation. Here, we tailor the microenvironment of RTP emitters and, thus, the photophysical characteristics of the emissive layer by blending different polymers. While the blending of PMMA550k with PS350k led to inhomogeneous films with insufficient photophysical properties, mixing of PS350k with PS40k allows the finetuning of the UV dose required to activate the RTP emission in the PLTs. By combining polymers with different physical characteristics, the local matrix rigidity, oxygen permeability, and intermolecular interactions can be varied in a controlled manner. The study demonstrates how polymer-host engineering provides a systematic route to modulate the characteristics of PLTs while maintaining their key characteristics.

[1] Gmelch et al., Science Advances 2019. aau7310

CPP 17.13 Mon 19:00 P5

Unraveling biodegradable phosphorescent emitters by combining quantum chemical simulations with photophysical spectroscopy — •Philipp Wieland, Iuliia Malakhova, Sebastian Reineke, and Sebastian Schellhammer — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden

Naturally derived organic emitters are required for the design of efficient biodegradable photonic devices. For instance, quinoline alkaloids exhibit sufficient emission via room-temperature phosphorescence (RTP), enabling their successful application in programmable luminescent tags for sustainable information storage [1]. Despite minimal structural differences between specific emitters of this quinoline alkaloid material family, they result in very different device performances.

In this work we present a combined experimental and computational characterization of RTP-active quinoline alkaloids, aiming to improve the understanding of their structure-property relationship. Photoluminescence analysis of quinine and cinchonine shows that phosphorescence dominates as the radiation process in cinchonine, whereas fluorescence is much more pronounced in quinine. To understand the origin of these differences, Density Functional Theory simulations are conducted. Conventional modelling approaches typically rely on static descriptions, which, while efficient, fail to capture the behavior of highly dynamic molecules. To overcome this limitation, we explicitly incorporate Molecular Dynamics into the screening of excited state properties. [1] Thomas et al. Adv. Mater. 2024, 36, 2310674.

CPP 17.14 Mon 19:00 P5

Stabilization via Confinement of Halide Perovskites — •Marius Kaiser[1], Osama Alsheika[2], Helen Grüninger[2], and Eva M. Herzig[1] — [1]Dynamik- und Strukturbildung - Herzig Group, University of Bayreuth, Germany — [2]Bavarian Center for Battery Technology (BayBatt) and Inorganic Chemistry, University of Bayreuth

The practical use of halide perovskites (HPs) for optoelectronic applications is severely limited by degradation caused by intense light exposure, heat, and unintended ion transport under external electric fields [1]. Key challenges in this field include understanding the underlying mechanisms, stabilizing the semiconductor, and achieving controlled electron and ion transport.

Methylammonium lead bromide (MAPbBr3) is used as a model system, and its lattice parameters are systematically investigated in both bulk form and when confined within SBA-15 silica nanopores (average diameter ~8.4 nm), across a range of temperatures and pore loadings.

Furthermore, we examine thermal expansion behaviour of the materials and evaluate the effect of surface functionalization.

These results provide valuable insights for the development of more stable HP-based optoelectronic devices with directionally controlled charge transport.

[1] Greve, C. et al. To Stop or to Shuttle Halides? The Role of an Ionic Liquid in Thermal Halide Mixing of Hybrid Perovskites. ACS Energy Lett. 8 (2023).

CPP 17.15 Mon 19:00 P5

Early-Stage Growth and Morphological Evolution of Ag Electrodes during Sputter Deposition on PDINN — •Doan Duy Ky Le[1], Kristian Reck[2], Benedikt Sochor[3], Thomas Strunskus[2], Jungui Zhou[3], Anuragk Keloth[3], Lyuyang Cheng[1], Sarathal Koyiloth Vayalil[3], Stephan V. Roth[3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]CAU, Kiel, Germany — [3]DESY, Hamburg, Germany

The integration of sputtered metal electrodes with organic interlayers remains a key challenge for the scalable fabrication of organic solar cells (OSCs). PDINN is an efficient cathode interlayer, yet its behavior under sputter deposition is not well understood. Here, we use *in situ* GISAXS to resolve the nanoscale morphological evolution of Ag during direct-current magnetron sputtering (DCMS) onto PDINN thin films. Time-resolved scattering reveals distinct early-stage growth regimes, including the nucleation of small Ag clusters, their coalescence into medium-sized species, and the formation of laterally connected domains. Compared to thermally evaporated Ag, sputtered Ag achieves continuous coverage at significantly reduced thickness. These findings confirm the feasibility of sputter-deposited Ag/PDINN interfaces and establish a foundation for scalable electrode fabrication in next-generation OSCs.

CPP 17.16 Mon 19:00 P5

Spin-Sensitive Spectroscopy of TADF OLEDs — •Andreas Kohrmann, Ahmed Mohamed, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

The performance of the blue emitter ν-DABNA in thermally activated delayed fluorescence (TADF) organic light-emitting diodes (OLEDs) is closely related to the dynamics of triplet excitons. In optically excited host-guest thin films, triplet states are generated and evolve through the intricate interplay of triplet diffusion, triplet recombination, and triplet-triplet annihilation (TTA). Thereby TTA and triplet diffusion are inherently host-dependent. Consequently, the host environment exerts a pivotal influence on exciton loss and delayed emission pathways. We used spin-sensitive optical spectroscopy, specifically photoluminescence-detected magnetic resonance (PLDMR) to examine the spin nature of the singlet-triplet interaction in optically excited host-guest thin films. Correlating these with exciton kinetics from transient photoluminescence (trPL) yields insights on the luminescence as well as the formation, diffusion, and annihilation of triplet excitons. The findings of this study offer a more profound understanding of the triplet harvesting mechanisms in TADF emitters. Additionally, they offer guidance for host selection strategies that are intended to enhance the efficiency and stability of the devices.

CPP 17.17 Mon 19:00 P5

Excimers in carbazole-substituted 4NICz TADF emitters: from frozen solution to films. — •Anatolii Kuimov[1], Oliver Lee[2], Eli Zysman-Colman[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth, 95440 Bayreuth, Germany. — [2]Organic Semiconductor Centre, EaStCHEM School of Chemistry, University of St Andrews, St Andrews, UK, KY16 9ST

To obtain high brightnesses in OLEDs, emitters need to be packed sufficiently densely for good charge transport. However, too close a proximity between chromophores can lead to the formation of excimers. We investigate under which conditions such excimers are formed in carbazole-substituted 4NICz blue emitters and how this formation can be controlled. In dilute solution at room temperature, we see only emission from non-interacting molecules, whereas in frozen glass a weak red-shifted emission band appears that grows with laser intensity. A similar increase is observed in films. We attribute excimer formation in the glass and in films to structural reorganization after local heating that results from the absorption of the laser pulses.

CPP 17.18 Mon 19:00 P5

Bulk-Heterojunction Morphology Engineering in D18:Y6 Solar Cells — •Dennis Straub, Lixing Li, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Organic solar cells based on non-fullerene acceptors have attracted considerable interest due to their favourable optoelectronic properties and compatibility with low-temperature solution processing. In this work, the D18 polymer donor and the non-fullerene acceptor Y6 (BTP-4F) are used as the active layer materials. The study investigates how variations in fabrication parameters influence the evolution of the bulk-heterojunction morphology and the resulting photovoltaic behaviour. Key factors examined include solvent choice, wet-film formation, drying kinetics, and thermal treatment, which govern phase separation, domain purity, and molecular ordering within the active layer.

To further explore morphology control, selected additives are introduced that may affect miscibility, aggregation, and domain formation. Their influence on the structural organisation of the D18:Y6 blend is analysed to determine how additive-induced morphological changes impact charge generation, transport pathways, and recombination processes. By correlating structural characteristics with device performance, this work aims to clarify how processing and material modification shape the efficiency and reproducibility of D18:Y6 organic solar cells and to provide guidance for future optimisation.

CPP 17.19 Mon 19:00 P5

Spray Engineering for High-Efficiency Organic Solar Cells — •Xinyu Jiang[1], Kang An[2], Nadja Koelpin[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

Spray coating has emerged as a powerful and scalable technique for fabricating high-performance organic solar cells (OSCs), offering precise control over ink deposition and rapid compatibility with large-area manufacturing. Compared with conventional solution-processing methods, spray deposition enables fine tuning of droplet dynamics, solvent evaporation, and wet-film thickness, which are critical for achieving optimal phase separation and molecular ordering in the active layer. In this work, we demonstrate that rational engineering of spray parameters such as atomization rate, nozzle substrate distance, carrier-gas flow, and solvent volatility significantly improves film uniformity and reduces morphological defects, leading to enhanced charge transport and suppressed recombination losses. By integrating these optimized spray processes, the resulting OSCs exhibit markedly improved device efficiency and excellent reproducibility across enlarged areas. These results highlight spray coating as a highly efficient and industry-ready pathway for the scalable integration of organic solar cells.

CPP 17.20 Mon 19:00 P5

Narrowband organic Photodetectors with J-Aggregate materials — •Angelina Stoer[1], Jakob Wolansky[1], Matthias Stolte[2], Frank Würthner[2], Karl Leo[1], and Johannes Benduhn[1] — [1]Institut für Angewandte Physik und Photonik, TU Dresden — [2]Institut für Organische Chemie, Universität Würzburg

With the development of organic photodetectors, new opportunities for narrowband photodetection have emerged. Instead of relying on costly and unwieldy optical filters, the molecular structure of organic materials can be chemically tailored to tune their absorption range. Recently, the material class of merocyanine dyes has been investigated as a promising candidate for this purpose, exhibiting favorable absorption properties. By post-annealing these dyes, the molecules can rearrange and form J-aggregated thin films, resulting in a narrowband absorption spectrum due to the intermolecular interactions.

In this work, the merocyanine dye 1(Hex) is used in fully vapor-deposited organic photodetectors. Narrowband detection with a FWHM as low as 15 nm could be realized at a center wavelength of 755 nm. Through careful optimization of the heating conditions and device structure, a notable external quantum efficiency was achieved, accompanied by very low noise at zero voltage. Based on this, the resulting specific detectivity exceeds 10^{12} Jones. The comprehensive photodetector characterization is complemented by an in-depth analysis of changes in the thin film‘s morphology and energetics induced by the J-aggregation formation process.

CPP 17.21 Mon 19:00 P5

Nanoscale Structural and Electronic Characterization of the DTDCPB:C70 donor-acceptor system for vacuum-deposited organic solar cells — •Milena Merkel[1,2], Jan ter Glane[1,2], and Harry Mönig[1,2] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Center for Nanotechnology (CeNTech), Münster, Germany

The active layer of organic solar cells is produced either by solution-processing or vacuum thermal evaporation. While solution-processed cells have achieved higher efficiencies to date, vacuum-deposited cells exhibit higher morphological stability and thus a longer durability. For a future commercialization of organic solar cells, where both efficiency and durability are crucial, understanding the current limitations of vacuum-deposited cells is thus of major interest.

Cells based on an active layer made of the DTDCPB:C70 donor-acceptor system have so far achieved one of the highest efficiencies in the group of vacuum-deposited organic solar cells, while also exhibiting high durability [1,2]. We used a combined approach of high-resolution scanning tunneling microscopy and spectroscopy to investigate the structural and electronic properties of assemblies of these donor and acceptor molecules deposited on single-crystalline substrates, as well as of their lateral and vertical interfaces.

[1] Griffith et al., Phys. Rev. B 92, 085404 (2015)
[2] Zou et al., J. Mater. Chem. A 2, 12397 (2014)

CPP 17.22 Mon 19:00 P5

Interfacial modification of transport layers for enhancing the performance and stability of organic solar cells — •Saib Jahan Qazi[1,2], Md. Moidul Islam[1,2], Md. Zobaer Ahmed Rahat[1,2], Md. Farhatul Hassan[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, lightweight 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 due to inherent instability particularly at the interfaces. In this study, we demonstrate solution processed interfacial modification of zinc oxide (ZnO). ZnO is widely used in organic solar cells for electron extraction, but it brings performance and lifetime limitations due to surface defects and photochemical reactions under UV exposure, which generates radicals resulting into accelerated degradation of the photoactive layer in the device. Here we compare approaches using organic acids with polysilazane, for successful ZnO passivation.

CPP 17.23 Mon 19:00 P5

Simulation of Pump-Probe Spectra Including Linear Vibronic Coupling – A Study on Naphthalene Diimide — •Matthias Knechtges, Maximilian F. X. Dorfner, and Frank Ortmann — Department of Chemistry, TUM School of Natural Sciences, and Atomistic Modeling Center, Munich Data Science Institute, Technical University of Munich, München, Germany

Non-linear optical techniques such as pump-probe spectroscopy provide insight into the dynamical processes governing excited-state evolution, which are often influenced by electron-vibrational interactions. The theoretical computation of pump-probe spectra remains an open research field [1] due to the complicated treatment of coupled electronic and nuclear dynamics, which require feasible but accurate approximations [2]. In particular, including the full quantum nature of the nuclei remains a major challenge.

In this contribution, we present a framework for calculating pump-probe spectra of molecules based on an analytic linear electron-vibrational coupling model. Evaluating the third-order response function in the Franck-Condon approximation and including vibrational transitions enables us to predict the pump-probe signal in the infrared region as well. We apply this to the Naphthalene Diimide molecule, a building block for a prospective solar cell material.

[1] Gelin, M., et al., Comp. Mol. Sc. (2025); [2] Park, J. W., et al., J. Chem. Theory Comput. (2017)

CPP 17.24 Mon 19:00 P5

QD-based hybrid organic photo detectors for narrowband IR sensing — •Johann Demel[1], Louis Conrad Winkler[1,3], Andrey Iodchik[2], Moritz Flemming[1], Tobias Antrack[1], Karl Leo[1], and Johannes Benduhn[1,3] — [1]IAP, TU Dresden — [2]Chemistry, TU Dresden — [3]German Center for Astrophysics

The ability to detect infrared radiation is relevant across a multitude of fields. Autonomous driving and deep space exploration utilize its ability to propagate long distances with little absorption losses. While, e.g., medical diagnostics can profit from its penetration depth into biological tissue. Organic materials have proven to be a viable platform for photo detection, with advantages such as low-cost fabrication, flexible devices, and tunable absorption; however, their IR absorption capabilities are limited.

This work presents a hybrid structure combining organic transport layers and PbS nanoparticles into optical microcavities. Based on transfer-matrix simulations, the resonance wavelength of the stack can be precisely predicted and tuned by adjusting the thickness of the organic transport layers. By combining precise thermal evaporation of the organic layers with interface assembly to incorporate nanoparticle layers into the stack, wavelength-selective devices are achieved whose resonance feature can be tuned from 750 nm up to 1800 nm. This expands the advantageous properties of the organic device framework by the wavelength-tunable IR absorption capabilities of semiconductor nanoparticles, leading to devices with specific detectivity values D^* of $10^{11}\ cm \cdot \sqrt{Hz} \cdot W^{-1}$ (based on noise measurements).

CPP 17.25 Mon 19:00 P5

Heat induced morphological changes in P3HT:PCBM solar cells — •Jose Prince Madalaimuthu[1,2], Edward Wijaya[1,2,3], Ulrich S Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller-Universität Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-Universität Jena, Germany — [3]Department of Chemical Engineering, Swiss German University, 15143 Tangerang, Indonesia

Organic solar cells are becoming an important technology for next-generation energy applications since they can be made into flexible and lightweight devices. However, attaining thermal stability remains a significant challenge for its actual deployment. Heat-induced morphological alterations within the photoactive layer typically led to considerable performance reductions. It's interesting to note that this effect may be reversed in some circumstances. Our investigations on P3HT:PCBM solar cells show that devices subjected to high-temperature exposure (up to 250°C) demonstrated substantial performance recovery upon cooling. Thermally driven and reversible morphological change in the active layer was demonstrated by photoluminescence analysis.

CPP 17.26 Mon 19:00 P5

Trace Intrinsically Microporous Polymer Additives Induce LiF-Rich SEI for Enhanced Performance of Silicon-Based Lithium-Ion Batteries — •Ming Yang[1], Ruoxuan Qi[1], Ya-Jun Cheng[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]College of Renewable Energy, Hohai University, Changzhou, Jiangsu Province, P. R. China

Silicon-carbon (Si/C) composite anodes are promising candidates for high-energy-density lithium-ion batteries due to the high theoretical capacity of silicon. However, their practical application is hindered by severe volume expansion and unstable solid electrolyte interphase (SEI) formation during cycling. Fluoroethylene carbonate (FEC) is commonly used to improve interfacial stability, but its effectiveness is limited by concentration sensitivity and uncontrollable side reactions. This study introduced carboxyl-functionalised intrinsically microporous polymer (PIM-COOH) as a functional additive, achieving dual regulation of electrode structural evolution and interfacial chemistry. Only 0.5wt% PIM-COOH is required to achieve these effects. The Si/C@PIM||Li half-cell retains 90% of its capacity after 300 cycles at 1.0 C, demonstrating excellent long-term stability. The utilisation of 1Ah NCM811-Si/C pouch cells demonstrates its commercial potential. These results demonstrate a scalable and effective strategy for stabilizing silicon-based anodes, offering valuable insight into the design of next-generation lithium-ion batteries with both high energy density and long cycle life.

CPP 17.27 Mon 19:00 P5

In-situ WAXS observation of 3D porous electrodeposition Cu in lithium-metal batteries — •Lyuyang Cheng[1], Zhuijun Xu[1], Yingying Yan[1], Fabian Apfelbeck[1], Yuxin Liang[1], Anton Davydok[3], Christina Krywka[3], Yajun 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 — [3]Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

Lithium (Li) metal is the ultimate anode for rechargeable batteries. Its high specific capacity (3860 mAh/kg) and low voltage warrant optimal cell energy density. However, these anodes rely on repeated plating and stripping of Li, which leads to consumption of Li and the growth of dendrites that can lead to self-discharge and safety issues. To address these issues and problems, 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 illustrate 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 17.28 Mon 19:00 P5

Ionic-Liquid-Regulated PVC-Based Solid Polymer Electrolyte for High-Performance Lithium Metal Batteries — •Jiaqi Ding and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Lithium metal batteries (LMBs) are regarded as one of the most promising next-generation energy-storage systems owing to their ultrahigh theoretical capacity. However, the safety issues associated with conventional liquid electrolytes, including dendrite-induced short circuits and interfacial instability, severely hinder their practical application. Solid polymer electrolytes (SPEs) offer a potential pathway to address these challenges. In this work, we develop a poly(vinyl carbonate) (PVC)-based solid polymer electrolyte incorporating the ionic liquid [EMI][TFSI] to enhance both ion transport and mechanical integrity. Structural and electrochemical characterizations show that the ionic liquid effectively regulates ion transport within the polymer matrix, enabling the formation of continuous Li ion conduction pathways and improving the compatibility of the electrolyte with lithium metal. This tailored ion-transport behavior leads to enhanced ionic conductivity, mitigated interfacial degradation, and significantly extended cycling stability in LMBs. The results highlight the critical role of ionic-liquid modification in tuning transport properties of polymer electrolytes and provide a viable materials strategy for high-performance lithium metal batteries.

CPP 17.29 Mon 19:00 P5

Investigation of the Effects of LiDFOB Salt Concentration on the Fast-Charging Performance of LiCoO2 Cathodes — •Yifeng Liu, Ming Yang, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Fast-charging lithium-ion batteries have drawn increasing interest, yet lithium cobalt oxide (LiCoO$_2$) paired with commercial electrolytes generally suffers from severe capacity fading and limited cycle life at high charging rates. This study aims to explore strategies for improving capacity retention of LiCoO$_2$-based lithium-ion batteries under fast-charging conditions. We employ boron-containing lithium salt LiDFOB as an electrolyte additive and systematically investigate its concentration-dependent effects on the capacity retention of LCO cells under fast-charging operation. Interfacial stability and charge-transfer kinetics associated with different LiDFOB levels are evaluated through cyclic voltammetry (CV), linear sweep voltammetry (LSV), Tafel analysis, and chronoamperometry (CA). The results show that the concentration of LiDFOB has a pronounced influence on the cycling performance. In particular, the optimized LiDFOB concentration enables the LCO cells to stably cycle for over 1000 cycles at 1C and 3C, benefiting from the improved interfacial stability and enhanced Li$^+$ transference number. Morphological and material characterizations further reveal that different LiDFOB concentrations generate SEI films with distinct compositions and structures, which account for the disparities in fast-charging capacity retention.

CPP 17.30 Mon 19:00 P5

High-Power Continuous Laser-Guided Synthesis of Bimetallic Metal-Organic Framework (NiCoMOF) Structures and Their Composites: Photophysical, Photochemical, and Electrical Characterization — •Saliha MUTLU[1,2], Bülend ORTAÇ[2], Ali KARATUTLU[2,3], Nergis ARSU[4], and Sevil SAVAŞKAN YILMAZ[1,2] — [1]Karadeniz Technical University Chemistry Department, Trabzon, Türkiye — [2]Bilkent University, Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM), Ankara, 06800 Turkey — [3]Sivas University of Science and Technology, Department of Engineering Basic Sciences, Sivas, 58100 Turkey — [4]Department of Chemistry, Yildiz Technical University, Davutpasa Campus, Istanbul 34210, Turkey;

Metal-organic frameworks (MOFs) are among the most innovative breakthroughs in chemistry and materials science. In this study, the first bimetallic synthesis of MOFs was achieved using the high-power laser-induced rapid synthesis (LIRS) method via two different ligand and metal salt combinations with different π-conjugated linkers. The synthesis of NiCo-MOF structures (in 1:2 and 2:1 ratios) was completed in just 70 minutes using the LIRS method. Furthermore, the synthesis of MOF composites (rGO/MOF) containing reduced graphene oxide (rGO) was also achieved for the first time. On top of these, the electrical properties of the epoxy acrylate-based MOF and rGO@MOF composites prepared by in situ photopolymerization were investigated in detail. This study was supported by TÜBITAK-BIDEB 2211-A National PhD Scholarship Programs.

CPP 17.31 Mon 19:00 P5

A gel polymer electrolyte interface layer-amphiphilic polymer/salt composite nanoarray for lithium metal batteries — •Thomas Bullinger, Ming Yang, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Research on lithium-ion batteries has been focused on improving energy density, which is mainly limited by conventional graphite anodes. Therefore, lithium metal has emerged as a desirable anode material due to its high energy density. However, it easily reacts during cycling, thus forming lithium dendrites, which can lead to short-circuiting of the battery. As liquid electrolytes cannot solve this problem, solid-state polymer electrolytes have shown promise as an alternative, but their ionic conductivity at room temperature limits their practical use, leading to the compromise of gel polymer electrolytes. In this project the block copolymer P2VP-b-PEO together with the lithium salt lithium nitrate, both dissolved in tetrahydrofuran (THF), surprisingly lead to the solvent phase changing to a gel polymer, which was then used as the electrolyte in coin cells. For the cycling and rate performance tests, Li||LFP batteries were investigated. Further experiments include cycling voltammetry (CV), linear sweep voltammetry (LSV), Tafel curves and impedance spectroscopy.

CPP 17.32 Mon 19:00 P5

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, 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 layer 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 17.33 Mon 19:00 P5

Effects of differently sized and shaped active and passive Filler for PVDF-HFP CPEs in All Solid-State Lithium-Ion Batteries — •Daniel Karlinger, Yuxin Liang, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Graching, Germany

All-solid-state lithium-ion batteries are regarded as highly promising due to their enhanced safety and potentially higher energy density compared to conventional cells with liquid electrolytes. In this project, solid polymer electrolytes based on PVDF-HFP are investigated with the aim of improving ionic conductivity and overall electrochemical performance. The approach is to incorporate combinations of ac tive and passive fillers to tailor the material properties. Conductivity and mechanical stability will be systematically examined with cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), X ray diffraction (XRD) and other methods, in order to identify optimized compositions for solid-state battery applications.

CPP 17.34 Mon 19:00 P5

Tracing the Path from Solvation to Transport in Lithium and Sodium Electrolytes — •Chinwendu Nancy Anabaraonye[1,2], Diddo Diddens[3], and Andreas Heuer[1,2] — [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]Forschungszentrum Jülich GmbH, Helmholtz-Institute Münster (IMD-4), Corrensstraße 48, 48149 Münster, Germany

Advancing technology continues to increase demands on energy storage devices and their performance requirements. Over the years, lithium-ion batteries have consistently remained the market leader. However, their long-term sustainability remains questionable due to the limited lithium reserves. Therefore, there is need for increased research toward alternative battery chemistries, among which are sodium-ion batteries. The present work is a comparative study of the transport properties of lithium hexafluorophosphate (LiPF6) and sodium hexafluorophosphate (NaPF6) in carbonate electrolytes consisting of ethylene carbonate (EC) and ethyl methyl carbonate (EMC). Based on molecular dynamics simulations, we analyse the influence of EC ratio and salt concentrations on the solvation structure with particular focus on the formation of contact ion pairs (CIP), solvent-seperated ion pairs (SSIP) and ion aggregates and how this correlates with the ionic transports within the systems.

CPP 17.35 Mon 19:00 P5

Modeling Electron Transfer at Electrode-Electrolyte Interfaces — •Joshua Krieger[1,2,3], Johannes Tölle[4,5,3], Diddo Diddens[2,6], and Andreas Heuer[2,6] — [1]International Graduate School BACCARA, University of Münster, 48149 Münster, Germany — [2]Institute for Physical Chemistry, University of Münster, Münster, Germany, 48149 Münster, Germany — [3]Center for Multiscale Theory and Computation (CMTC), University of Münster, 48149 Münster, Germany — [4]Department of Chemistry, University of Hamburg, 22761 Hamburg, Germany — [5]The Hamburg Centre for Ultrafast Imaging (CUI), 22761 Hamburg, Germany — [6]Helmholtz Institute Münster - Forschungszentrum Jülich GmbH (IEK 12), 48149 Münster, Germany

The solid electrolyte interphase (SEI) is an important component in rechargeable battery performance and lifetime, but the complex mechanisms behind its formation are still not yet fully understood. Accurate electron-transfer (ET) rates are important for simulating SEI growth, e.g. using reactive molecular dynamics simulations that require electrolyte reduction rates. To obtain the ET rates, we investigate a simplified Anderson impurity-type model designed to describe non-equilibrium electron transfer between an electrode and the redox-active species under an applied potential. This framework enables systematic exploration of how molecular distance, electronic coupling, as well as solvent interactions and reorganization effects influence electron-transfer dynamics. The resulting insights provide a foundation for constructing more reliable, physics-based rate expressions that can be integrated into large-scale SEI formation simulations.

CPP 17.36 Mon 19:00 P5

Toward Improved Lithium Batteries: Performance of Magnetron-Sputtered Silicon Anodes — •Thomas Köhler[1], Christian Ludt[1], Tina Weigel[1], Marc Ferch[2], Robert Hahn[2], Annekatrin Delan[3], Charaf Cherkouk[4], Hartmut Stöcker[1], and Dirk C. Meyer[1] — [1]TU Bergakademie Freiberg, 09599 Freiberg, Germany — [2]Fraunhofer IZM, 13355 Berlin, Germany — [3]Fraunhofer IZM-ASSID, 01468 Moritzburg, Germany — [4]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Silicon is considered one of the most promising anode materials for lithium-ion batteries due to its high theoretical specific capacity of 3590 mAh/g in the Li$_{3.73}$Si phase at room temperature and its broad availability. However, its practical application remains limited because i) significant volume changes occur during cycling, ii) its intrinsic electronic conductivity is low, and iii) the stability of the solid-electrolyte interphase is insufficient.

In this work, silicon thin-film anodes were fabricated by magnetron sputtering onto copper foil. The electrodes were thoroughly characterized regarding their chemical composition and surface morphology. Scanning electron microscopy was used to evaluate the structural stability of the silicon layers in contact with a polymer-based solid electrolyte and to compare their degradation behavior with that in conventional liquid electrolyte. Electrochemical testing with the polymer electrolyte shows promising cycling performance; the reduced surface degradation observed in SEM correlates with improved long-term stability of the cell system.

CPP 17.37 Mon 19:00 P5

Structural and Ionic Transport Properties of Li3-3xDy1+xCl6 Solid Electrolytes — •Francesco Falsina[1,2], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]MLZ, TUM, Garching, Germany

Ternary lithium lanthanide chlorides, Li$_3$RCl$_6$ (R = rare earth), have recently emerged as promising solid electrolytes. Although initially thought to exhibit low ionic conductivity, later studies showed that ball milling synthesis, by leading to microstructure modification, can raise conductivity to $\sim 10^{-3}$ S·cm^{-1}. In this work we studied the Li$_{3-3x}$Dy$_{1+x}$Cl$_6$ system (x = −0.1 to 0.1). For $x = 0$, we assessed how annealing conditions affect structure and conductivity. Ionic transport was measured using isostatically pressed, gold-sputtered pellets and broadband impedance spectroscopy. XRD, DSC, and EIS analyses of as-milled, annealed, and melt-synthesized samples show that conductivity decreases by nearly an order of magnitude after annealing, while over-lithiated compositions consistently display higher conductivity, highlighting the impact of lithium retention. DSC and XRD also reveal an orthorhombic-to-trigonal transition with increasing lithium content. Overall, these results clarify how composition and disorder govern ionic transport in the Li$_3$MCl$_6$ electrolyte family.

CPP 17.38 Mon 19:00 P5

Investigating the Interfacial Impedance Characteristics of Composite Materials — •Janne Mattis König[1,2], Felix Schug[1,2], Christian Heiliger[1,2], and Janis K. Eckhardt[1,2,3] — [1]Institute of Theoretical Physics, Justus-Liebig-University Giessen, 35392 Giessen, Germany — [2]Center of Material 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 a promising alternative to conventional lithium-ion batteries, offering high energy and power densities, long-term stability, and fast-charging capability. Consequently, significant effort is focused on identifying suitable materials. Electrochemical impedance spectroscopy (EIS) is a key characterization technique, but interpreting spectra from realistic composite systems remains challenging. In this work, we investigate interfacial impedance in simplified composite microstructures using a 3D electrical network model. The simulations reveal that high charge-transfer resistances lead to geometric constriction effects, producing an impedance signature that closely resembles a migration process or a charge-transfer reaction. This constriction impedance is strongly influenced by the composite microstructure. Furthermore, increased conductivity along the interface introduces a characteristic deformation in the impedance spectrum shape. Overall, these findings clarify the origin of interfacial impedance features in composite materials and support more informed interpretation of EIS measurements in ASSB research.

CPP 17.39 Mon 19:00 P5

Aluminium-Polymer Batteries as a viable Post-Lithium Technology — •Oliver Schmidt[1,2], Amir Mohammad[1,2], Shuvrodev Biswas[1,2], Mostafizar Rahman[1,2], Nathan Leubner[1,2], Thomas Köhler[1,2], Hartmut Stöcker[1,2], and Dirk C. Meyer[1,2] — [1]TU Bergakademie Freiberg, Institute of Experimental Physics, Leipziger Str. 23, 09599 Freiberg — [2]Zentrum für effiziente Hochtemperatur-Stoffwandlung, Winklerstr. 5, 09599 Freiberg

One of the key challenges of the energy transition is the rising demand for lithium. In the future, there will be a supply gap, even taking into account recycling and the development of new mining areas. In addition to the limited availability, safety risks such as fire hazards make lithium-ion batteries less suitable for the long-term requirements of the energy transition.

Here, we present the aluminium-polymer battery as a novel technology adressing these issues. Aluminium is the most abundant metal in the Earth's crust and therefore inexpensive. It is available in Europe and is highly recyclable. The battery cells are free of toxic or critical raw materials and eliminate the risk of fire.

Pouch cells consisting of a simple 3-layer setup have been developed: aluminium anode, polymer electrolyte (consisting of AlCl$_3$, Et$_3$NHCl and PAN) and graphite cathode. Capacity, safety and recycling tests show promising results. Remaining challenges are tackling the self-discharge and scaling up the cell fabrication. The future goal is making large-scale storage systems cost-effective, efficient and safe.

CPP 17.40 Mon 19:00 P5

Microstructure-Resolved Impedance Modeling of Cathode Composite Electrodes for Solid-State Batteries — •Matthias Braun[1,2], Felix Schug[1,2], Christian Heiliger[1,2], and Janis K. Eckhardt[1,2,3] — [1]Institute for Theoretical Physics, Justus-Liebig-University Giessen, Germany — [2]Center for Materials Research (ZfM), Justus-Liebig-University Giessen, Germany — [3]Institute of Physical Chemistry, Justus-Liebig-University Giessen, Germany

Solid-state batteries (SSBs) rely on composite cathodes whose complex microstructures critically influence ionic and electronic transport. Electrochemical impedance spectroscopy (EIS) is widely used to probe these transport processes. The impedance behavior of mixed ionic electronic conductors is commonly interpreted using transmission-line models (TLMs). However, the extent to which composite microstructure governs impedance features and the validity of TLM-based interpretations remains insufficiently understood. In this work, we employ microstructure-resolved impedance simulations to investigate how key structural characteristics of cathode composites shape their impedance response. We demonstrate that interface morphology and porosity significantly modulate the spectra, giving rise to microstructure-specific features that conventional TLMs fail to capture. In particular, geometric current-constriction effects at the cathode active material/solid-electrolyte interface emerge as dominant contributors to impedance behavior. These findings provide a deeper mechanistic understanding of microstructure-induced impedance signatures and offer practical guidance for interpreting EIS data in composite electrodes for SSBs.

CPP 17.41 Mon 19:00 P5

Optimization in Fabrication Process and Understanding the Impact of Crystal Size and Growth in RbCsMAFA Perovskite Solar Cells — •Bashudev Bhandari[1,2,3], Sai Durga Prasad Sudana[1,2], 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, Germany — [2]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller- University Jena, Germany — [3]Faculty of Physics and Astronomy, Friedrich-Schiller- University Jena, Germany

Perovskite solar cells (PSCs) emerged as remarkable and promising cutting-edge clean and green energy sources. Recent breakthroughs in their performance attract researcher's interest. Despite its promising performance, degradation issues and defects are critical obstacles to overcome. Our work explores different mechanisms to suppress defects and improve stability via improved crystallization. We have systematically optimized different processing parameters such as annealing time, antisolvent dropping time, hot casting, etc., and introduced additives like different phosphonium salts and PEAI for passivation and seeding for perovskite growth. Different Characterization and imaging techniques illustrate improved crystalline and opto-electronic properties of the perovskite film and solar cells.

CPP 17.42 Mon 19:00 P5

In Situ Investigation of Ag Sputter Deposition on a Zwitterionic Polymer Film — •Georgios Panagiotidis[1], Christoph Lindenmeir[1], Grace Leone[2], Lixing Li[1], Lyuyang Cheng[1], Doan Le[1], Yufeng Zhai[3], Kristian Reck[4], Benedikt Sochor[3], Matthias Schwartzkorpf[3], Anurag Keloth[5], Sarathlal Vayalil[3,5], Todd Emrick[2], Thomas Russell[2,6], Stephan V. Roth[3,7], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]UMass Amherst, Massachusetts, United States — [3]DESY, Hamburg — [4]CAU, Kiel, Germany — [5]UPES, Dehradun, India — [6]LBNL, Berkeley — [7]KTH, Stockholm, Sweden

While organic electronic devices mainly use organic or organic-inorganic hybrid materials, many electrodes still rely on pure metals due to their unparalleled electrical conductivity. Thus, the polymer-metal interface is crucial to device performance. Studies have demonstrated the use of ultrathin metal electrodes for (semi)transparent organic solar cells, and the quality of the interface influences the formation of structural defects, which can increase resistance and the likelihood of a short circuit. These metal contacts are typically deposited through lab-scale methods such as thermal evaporation, while industrial manufacturing prefers large-scale sputter deposition. Moreover, zwitterionic polymers can reduce the work function of metals and serve as interlayers in inverted organic solar cells. Therefore, understanding the growth behavior of sputtered silver on zwitterionic polymer surfaces is critical.

CPP 17.43 Mon 19:00 P5

Probing the Distribution of Residual Stresses in Thin Polymer Films Using Mechanochromic Molecular Springs — •Meirui Fu[1], Raphael Hertel[2], Bence Dajka[3], Michael Walter[3], Michael Sommer[2], and Günter Reiter[1] — [1]Institute of Physics, University of Freiburg, Germany — [2]Institute for Chemistry, Chemnitz University of Technology, Germany — [3]FIT Freiburg, University of Freiburg, Germany

Polymer thin films prepared rapidly from solution by spin coating often retain residual stresses originating on a molecular level. However, typically these stresses are probed on a macroscopic level, yielding spatially averaged responses, but do not resolve forces acting on individual chains. Here, we employed mechanochromophores, covalently integrated along the backbone of a glassy polymer, as optical reporters whose emission response varies continuously with the applied force. By combining optical microscopy and spectroscopy, we were able to measure the sum of the forces acting on individual chains with high spatial resolution. In particular, we investigated the distribution of forces acting on non-equilibrated polymer chains. Samples prepared under different spin coating conditions exhibited systematic variations in the emission spectra, which reflect differences in the distribution of the sum of forces acting on individual chains. We distinguish contributions from polymers experiencing low and high forces, respectively, which exhibited opposite trends with preparation conditions. We tentatively relate the heterogeneity of the acting forces to differences in conformation of the non-equilibrated polymer chains.

CPP 17.44 Mon 19:00 P5

Real Time Spectroscopy of Plasmonic Core-Shell Microgels during Compression at Air/Water Interfaces — •Matthias Karg and Déborah Feller — Martin Luther University Halle-Wittenberg, Halle, Germany

Plasmon resonance coupling is strongly distance-dependent. In contrast to near-field coupling of plasmonic nanoparticles in close proximity, periodic superstructures support plasmonic-diffractive coupling. The resulting surface lattice resonances are interesting for their narrow linewidth and sensitivity to refractive index environment and lattice periodicity. Typically studied periodic arrays are (solid) substrate-supported and thus structurally fixed unless elastic substrates are used. Seeking an alternative approach, we demonstrate the large dynamic control of periodic plasmonic lattices using soft and deformable core-shell microgels self-assembled at air/water interfaces. Using microgels with gold cores and sufficiently thick microgel shells, we realized periodic monolayers where the periodicity can be controlled by compression using a Langmuir trough. The implementation of an extinction spectrometer setup was used to probe the optical response of the monolayer in situ during continuous reduction of the available area, in real time. We monitor plasmon resonance coupling with a never before reported stepsize in interparticle spacing by following peak position, width and intensity. The observed spectral changes support recent findings that confined microgel monolayers at fluid interfaces show a continuous reduction in spacing when uniaxially compressed opposed to the cluster formation that is observed after drying on solid substrates.

CPP 17.45 Mon 19:00 P5

In-situ FTIR spectroscopy on organic semiconductor electric double-layer transistors — •Marvin Schmidt[1], Pushi Wang[2], Jun Takeya[2,3], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Graduate School of Frontier Sciences, The University of Tokyo, Kashiwa, Japan — [3]Research Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Japan

The field of organic electronics is ever-growing due to the enormous range of unique properties and possible applications exhibited by organic molecules. Electric double-layer transistors (EDLTs) consisting of the organic semiconductor 3,11-dinonyldinaphtho[2,3-*d*:2′,3′-*d*′]benzo[1,2-*b*:4,5-*b*′]dithiophene (C_9-DNBDT-NW) have recently attracted attention because they are highly processable and, thus, allow for the fabrication of large-scale single-crystal transistors with excellent crystallinity and high mobility. Furthermore, Hall effect measurements indicate the emergence of a metallic phase with strong correlations upon doping.

Here, we performed, for the first time, in-situ Fourier-transform infrared spectroscopy on EDLTs composed of C_9-DNBDT-NW single crystals for different sheet conductivities and temperatures down to 6K in the mid and far infrared regions. Our results give insights into how thermal fluctuations are suppressed with decreasing temperature and increasing electrostatic doping concentration, which manifests itself in the behavior of the displaced Drude peak.

CPP 17.46 Mon 19:00 P5

Measurement of photon antibunching of organic molecules by substrate scanning — •Janne Oskar Becker, Robert Schmidt, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics, University of Münster

Single-molecule photoluminescence spectroscopy is often performed in solution, with molecules drifting in and out of a stationary focus. To immobilize single molecules, they are typically diluted in a solvent and spin-coated on a substrate. However, bleaching processes lead to decreasing photoluminescence count rates when illuminating isolated single-molecules over time, making photon antibunching measurements extremely challenging. To circumvent this, we measure multiple molecules sequentially by spatially scanning the spin-coated surface and accumulating photons of multiple single-molecules. In that way, we are able to measure photon antibunching Si/SiO_2 substrate.

CPP 17.47 Mon 19:00 P5

Large-Area Semiconducting 2D Imine-COF Polymer Films on Dielectric Glass for Electronic Applications — •Diksha Srivastava[1], Vipin Mishra[2], Showkat H. Mir[3], Jyotirban Dey[1], Jayant k. Singh[1], Manabendra Chandra[1], and Thiruvancheril g. Gopakumar[1] — [1]Indian Institute of Technology Kanpur, Kanpur 208016, India — [2]Vellore Institute of Technology, Vellore, Tamil Nadu 632014, India — [3]University of Kashmir, Hazratbal, Srinagar 190006, Jammu and Kashmir, India

Two-dimensional imine-based covalent organic frameworks (2D COFs) are a growing class of crystalline π-conjugated organic polymers with strong potential in thin-film electronics and optoelectronics. We present a scalable and reproducible strategy for producing 2D imine-COF-based polymer thin films through a quasi-equilibrium Schiff-base reaction between p-phenylenediamine (PDA) and benzene-1,3,5-tricarboxaldehyde (TCA). This method enables the growth of large-area polymer films (up to 2 cm) on dielectric substrates with controlled thickness. SEM, TEM, and AFM confirmed the layered and crystalline morphology of the films. Optical absorption and scattering measurements revealed a semiconducting band gap consistent with the DFT-calculated band structures, indicating the presence of delocalized states suitable for charge transport. To probe intrinsic electrical behaviour, COF polymer films were integrated into Ag/COF/Glass devices. The I-V curves revealed semiconducting behaviour with low current density and field-assisted conduction limited by electrode-COF injection barriers.

CPP 17.48 Mon 19:00 P5

Designing functional polymer surfaces by initiated chemical vapor deposition — •Stefan Schröder, Lynn Schwäke, Tobias Giez, Thomas Strunskus, Franz Faupel, and Tayebeh Ameri — Kiel University, Kiel, Germany

Polymer thin films and organic surfaces have attracted significant interest across diverse application areas, ranging from wearable electronics to biomedicine and encapsulation. The demand for new functional surfaces, combined with ongoing device miniaturization, requires defect-free nanoscale polymer films with precise control over thickness and chemistry. Chemical vapor deposition (CVD) of polymer surfaces addresses these challenges by eliminating the dewetting and surface tension effects commonly encountered in conventional solution-based thin film fabrication. In particular, initiated chemical vapor deposition (iCVD) enables the fabrication of conformal polymer coatings with nanoscale precision on large-area substrates as well as on complex geometries. Moreover, iCVD allows for room-temperature deposition on delicate substrates, including flexible organic materials, copy paper, and biomedical patches. This contribution presents the fundamentals of the iCVD process and highlights selected application examples.

CPP 17.49 Mon 19:00 P5

Controlling Surface Wetting through Light- and Electric-Fields — •Billura Shakhayeva[1], Bas ter Beest[2], Frieder Mugele[2], and Björn Braunschweig[1] — [1]University of Münster, Institute of Physical Chemistry, Germany — [2]University of Twente, Physics of Complex Fluids

Electro-dewetting (EDeW) enables reversible control of surface wettability using ionic surfactants. Using dodecyl tetraethyl ammonium bromide (DTAB) as a cationic surfactant, previous studies achieved a change in the apparent contact angle (CA) of up to 30°. We used vibrational sum-frequency generation (SFG) spectroscopy and ellipsometry to probe the molecular structure close to the three-phase contact line under initial and EDeW conditions. Using 0.15 mM DTAB we observed the largest changes in contact angle and observed spreading of surfactant even at larger distances from the contact line. Further, we extended this approach from DTAB to photoswitchable arylazopyrazole triethylammonium bromide (AAP-TB) surfactants. AAP-TB can undergo E/Z photoisomerization and allows to change the surface activity through the choice of the configurational isomer with the Z being less surface active compared to the E. We demonstrate that EDeW with AAP-TB surfactants is possible similar to DTAB, but with a smaller maximum change in contact of about 13° once a potential of +3 V is applied. In addition, photo-isomerization of AAP-TB allows to further finetune the CA reversibly by about 4°.

CPP 17.50 Mon 19:00 P5

Dynamic wetting of mixed rod-sphere suspensions and its relation to the suspension rheology — •Reza Azizmalayeri and Günter Auernhammer — Leibniz-Institut für Polymerforschung Dresden e. V.

In this study, we examine dynamic wetting of mixed rod-sphere suspensions near the advancing contact line. We compare pure spherical suspensions with 98:2 sphere-rod mixtures. Using a pinned droplet and moving substrate geometry on an inverted microscope, we achieve a locally stable contact line. Astigmatism Particle Tracking Velocimetry (APTV) measures the trajectories of tracer particles within the refractive index-matched suspension. Pinch-off experiments conducted via the Dripping-onto-Substrate (DoS) method provide Protorheology insights into shear and extensional viscosities. We analyse rod dynamics and orientation as they approach the advancing contact line, interact with the substrate, and re-enter the bulk suspension. In purely spherical suspensions, tracer trajectories near the advancing contact line deviate significantly from hydrodynamic model predictions. Conversely, mixed rod-sphere suspensions exhibit minimal deviations. Rod inclusion reduces effective viscosity during pinch-off, promoting deformation and thread thinning. This effect is amplified by rod-induced polydispersity and the disruption of spherical contact structures, weakening resistance to flow and altering rheology. Visualizations reveal that rods align parallel to the contact line, then rotate 90 degrees to align with the substrate.

CPP 17.51 Mon 19:00 P5

Statics and dynamics of drops on liquid infused surfaces — Hossein Abdolnezhad[1], •Martin Brinkmann[2], Ralf Seemann[2], and Ciro Semprebon[1] — [1]Department of Mathematics, Physics and Electrical Engineering, Northumbria University, Newcastle, UK — [2]Zentrum für Biophysik, Universität des Saarlandes, Saarbrücken, Germany

Slippery liquid-infused porous surfaces (SLIPS), inspired by the slippery properties of the Nepenthes pitcher plant, have been introduced to increase the mobility of wetting drops by minimizing the liquid-solid contact. Preparation of these surfaces involves infusing a lubricating liquid into a porous or textured surface, creating a thin liquid layer on top of the surface resulting in high drop mobility as well as unique properties such as anti-corrosion, self-cleaning, heat transfer enhancing, anti-fouling and anti-icing, water harvesting properties with a broad potential for application in industry.

The complex relationship between lubricant properties and retention mechanisms in liquid-infused surface, particularly the role of the lubrication ridge forming around the drop causing depletion of the lubricant over time brings up the questions of whether the lubricant ridge can be effectively controlled as well as whether there is an optimal size in relation to the volume of the drop sliding over liquid-infused surface. Recent experiments elucidate the role of the lubricant ridge in the dynamics of drops on liquid-infused surfaces, and led to the development of a theoretical understanding of the experimental observations combining finite-element and analytical modeling approaches.

CPP 18: Active Matter III (joint session BP/CPP/DY)

Time: Tuesday 9:30–12:45 Location: BAR/SCHÖ

CPP 18.1 Tue 9:30 BAR/SCHÖ

inertia-driven re-entrant coil-Globule transition of active ring polymers — •Sunil P Singh[1], Roland G Winkler[2], Rakesh Palariya[1], and Arindam Panda[1] — [1]Indian Institute of Science Education and Research Bhopal, India — [2]Theoretical Physics of Living Matter, Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Germany

The role of inertia in the collective dynamics of active systems has been a subject of increasing interest in recent studies. The present study investigates the inertial effects on active agents. We present the conformational and dynamical characteristics of an active Brownian ring polymer using Langevin dynamics simulations. We show that a long active ring polymer shrinks into globular-like structures even in the absence of attractive interactions. This transition becomes sharper and the structures more compressed as the reduced moment of inertia of the monomers increases, particularly in the intermediate range of activity. We demonstrate that the ring polymer undergoes a coil-globule-coil transition, which is modulated by both activity and rotational inertia. The coil-to-globule transition is mapped in the inertial parameter space (J-M) using the radius of gyration. Additional physical quantities, including bond-bond correlations, scaling behavior in the compressed state, monomer contact probability, geometric distances, coordination number, and effective temperature, further elucidate the physical mechanism driving the collapse. Finally, we show that the effective diffusivity of the ring polymer increases with the reduced moment of inertia as $D_p \sim \sqrt{J}$.

CPP 18.2 Tue 9:45 BAR/SCHÖ

Shape selectivity by complex buckling dynamics in poroelastic active gels — •Kinjal Dasbiswas[1], Subhaya Bose[1], Arnab Roy[1], Michael Vennettilli[1], and Anne Bernheim[2] — [1]University of California, Merced, USA — [2]Ben Gurion University, Israel

Shape change in animal cells is prototypically driven by active forces, generated by myosin molecular motors bound to the actin cytoskeleton. Inspired by experiments on disc-shaped extracts of crosslinked actomyosin gels, we aim to show how a family of 3D shapes can arise from buckling caused by non-uniform active stresses. Although synthesized with identical composition of actin, myosin and the crossliker fascin, these gels contract and buckle into different shapes depending on the initial aspect ratio of the disc: thinner gels tend to wrinkle, while thicker gels tend to form domes. By incorporating active stresses, actin alignment, and stress-dependent myosin binding kinetics into a 2D poroelastic gel model, we qualitatively capture trends in gel contraction dynamics observed from quantitative particle image velocimetry (PIV). Next, we carry out numeric simulations of a geometric elastic model for thin sheets to obtain 3D buckled shapes from the strain rates predicted by the poroelastic model. Our results show that the coupling of elasticity to solvent flow, motor binding and fiber alignment play an important role in shape changes in living matter. Our studies have implications for shape changes during tissue morphogenesis and cell migration.

CPP 18.3 Tue 10:00 BAR/SCHÖ

The energy cost to build a spindle — •Dongliang Zhang[1], Xingbo Yang[4], Jan Brugués[2,1,3,4], and Frank Jülicher[1,3,4] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Center for Systems Biology Dresden, Dresden, Germany — [4]Physics of Life, Cluster of Excellence, TU Dresden, Dresden, Germany

Spindle is a structure actively build from microtubules (MTs), and plays an important role for chromosome segregation during cell cycle. It's observed in experiments that the spindle size and shape depends on the cell level metabolic rate. In this work, we developed a minimal model that captures the active, energy-consuming processes such as MT turnover and active stress generation, which shows the energy cost for spindle mass maintenance and spindle-shape formation. We show that a spindle can be self-organized through these active processes. We aim to predict how the size and shape of the spindle depends on the energy input, and explain relative experimental phenomena, e.g. spindle shrinkage when the metabolism level is reduced.

CPP 18.4 Tue 10:15 BAR/SCHÖ

Cytoskeletal oscillations drive large-scale flows and nuclear organization in early embryonic systems. — •Lara Koehler, Elissavet Sandaltzopoulou, and Jan Brugués — Physics Of Life, TU Dresden

Synchronization drives early embryonic development, enabling simultaneous cell divisions and the spatial organization of nuclei within the embryo. In organisms such as Xenopus, Drosophila, and zebrafish, mitotic waves coordinate cell cycles across distances that exceed diffusion limits, guided by a chemical oscillator. At the same time, global cytoplasmic flows in these syncytial tissues contribute to the large-scale self-organization of nuclei, yet the coupling between biochemical signaling and cytoskeletal mechanics that underlies these directed flows remains poorly understood. Here, we relax the geometric constraints of the embryo and investigate nuclear dynamics in Xenopus egg extracts and complementary simulations. We show that the periodic polymerization and depolymerization of microtubule asters are sufficient to generate robust large-scale directed flows, even though the asters are intrinsically isotropic. Furthermore, we demonstrate that cell division stabilizes short-range order in a global synchronized system. Together, these findings reveal a minimal physical mechanism by which cytoskeletal dynamics and biochemical oscillations jointly organize flows and patterns, with implications for understanding the emergent principles that shape early development across species.

CPP 18.5 Tue 10:30 BAR/SCHÖ

Geometric control of cell migration in disordered porous media — •Laeschkir Würthner[1] and Frederik Graw[2] — [1]European Molecular Biology Laboratory, Heidelberg, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg and Universitätsklinikum Erlangen, Erlangen, Germany

Cell migration is a dynamic process that plays a central role in development, wound healing, and immune responses. Active cell movement is controlled by several biochemical and mechanical cues, including chemokine gradients and the mechanical properties of the extracellular matrix (ECM). Although the biochemical pathways underlying directed cell motion are increasingly well understood, the influence of the porous structure of the ECM on active cell motion remains largely unexplored. Using a combination of computational modeling and theory, we investigate how active cells move through 3D disordered porous environments. We show that cell migration in disordered porous media can be understood as a generalized random walk among ”traps”, with the effective diffusivity determined by the geometry of the microenvironment. A key implication of our work is that spatial heterogeneities in porosity effectively direct cell motion, revealing a guidance mechanism that we refer to as porotaxis. Overall, our work connects geometry with cell motility and underscores the microenvironment as a key regulator of cell migration.

CPP 18.6 Tue 10:45 BAR/SCHÖ

Motility-induced mixing transition in exponentially growing multicellular spheroids — •Torben Sunkel[1,2], Lukas Hupe[1,2], and Philip Bittihn[1,2] — [1]MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

Growth drives cellular dynamics in various dense aggregates, but its effects on other relevant activities have only received limited attention. Here, we investigate the interplay of unconstrained growth, steric repulsion and motility in a minimal agent-based model of exponentially growing, three-dimensional spheroids. Our results reveal a diverging mixing time scale at a critical motility threshold, below which mixing of cells is completely suppressed. Above the threshold, large-scale mixing is enabled. Using an effective phenomenological model parameterized from full simulations, we identify two fundamental mechanisms governing this transition: On the cell scale, weak motility-induced active motion is locally suppressed by growth-induced steric repulsion, consistent with an Active Brownian Particle type description of single-cell dynamics. Beyond this, the expanding nature of the system inhibits global mixing purely geometrically by limiting the exploration range of diffusive cell motion. Both mechanisms naturally scale with the growth rate, highlighting the nature of the transition as an interplay between proliferation and motility. The results provide a baseline for identifying additional biological mechanisms in experiments and could be relevant for competition, heterogeneous tumor evolution and other manifestations of motile proliferating active matter.

15 min. break

CPP 18.7 Tue 11:15 BAR/SCHÖ

Fluctuation-Response Theory of Non-Equilibrium Complex Fluids — •Ryota Takaki[1] and Frank Jülicher[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, TU Dresden, Dresden, Germany

Active soft materials such as cytoplasm and tissues are constantly driven by chemical reactions and often retain long-lived mechanical memory. In this work, we develop a generalized hydrodynamic framework applicable to non-equilibrium fluids with memory at finite wavevectors and frequencies. Our approach is based on exact correlation-function identities, leading to a fluctuation-response relation for steady states, including non-equilibrium. Applying the theory to chemically driven active fluids, we uncover Active Viscoelastic Memory, in which reaction cycles dynamically renormalize the viscous response and can generate negative storage moduli at finite frequency, absent in conventional viscoelastic materials. Our results provide a first-principles basis for modeling memory-dependent dynamics in a broad class of biological and synthetic active systems, and suggest concrete rheological signatures of chemical driving that can be tested experimentally.

CPP 18.8 Tue 11:30 BAR/SCHÖ

Chemically Active Liquid Bridges Generate Repulsive Forces — •Noah Ziethen — DAMTP, University of Cambridge, UK

Intracellular droplets help organize cells by compartmentalizing biomolecules and mediating mechanical interactions. When such droplets bridge two structures, they generate capillary forces that depend on the surface properties and the separation between the structures. While the forces exerted by passive liquid bridges are well understood, the impact of active chemical reactions, ubiquitous in biological condensates, remains unclear.

Here, we investigate a single liquid bridge with continuous chemical turnover, in which the production and degradation of droplet material maintain a non-equilibrium steady state. In this active bridge, the reactions dynamically set the bridge radius, thereby controlling the force-distance relation. In striking contrast to passive systems, we find that activity can generate purely repulsive forces over a broad range of separations. These results show that chemical activity can qualitatively alter capillary forces generated by liquid bridges, suggesting a potential route for cells to actively regulate mechanical coupling via droplets.

CPP 18.9 Tue 11:45 BAR/SCHÖ

Shared Laws of Pattern Formation in Reaction-Diffusion and Phase Separation — •Daniel Zhou[1] and Erwin Frey[1,2] — [1]Arnold Sommerfeld Center for Theoretical Physics — [2]Max Planck School Matter to Life

Many nonlinear field theories generate a strikingly similar repertoire of patterns: arrested coarsening, traveling waves, and spatiotemporal chaos appear both in phase-separating systems and in classical reaction-diffusion models. These descriptions have different physical origins, yet recent studies on Turing mixtures and foams in protein systems [1] and on chemotaxis-driven phase separation in cell populations [2] have already highlighted unexpected connections between these ostensibly different mechanisms, linking foam-like, phase-separating, and reaction-diffusion-type patterns. The present work revisits the relation between kinetic and phase-separating descriptions from a more general viewpoint. A unifying perspective is developed that places different modeling frameworks on comparable footing, identifies the conditions under which they yield effectively equivalent patterns, and suggests how stability criteria and design principles can be translated between them. This points toward a more systematic classification of pattern-forming dynamics that cuts across traditional divides between reaction-diffusion, chemotactic, and phase-separating systems.

[1] H. Weyer et. al, Deciphering the Interface Laws of Turing Mixtures and Foams, arXiv:2409.20070 (2024).

[2] H. Weyer et. al, Chemotaxis-Induced Phase Separation, Physical Review Letters 135, 208402 (2025).

CPP 18.10 Tue 12:00 BAR/SCHÖ

Spatial self-organization of enzymes in complex reaction networks — •Vincent Ouazan-Reboul[1,2], Ramin Golestanian[2,3], and Jaime Agudo-Canalejo[2,4] — [1]LPTMS, CNRS, Université Paris-Sud, 91400, Orsay, France — [2]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, D-37077, Göttingen, Germany — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, OX1 3PU, Oxford, UK — [4]Department of Physics and Astronomy, University College London, WC1E 6BT, London, UK

Living systems contain intricate biochemical networks whose structure is closely related to their function and allows them to exhibit robust behavior in the presence of external stimuli. Such networks typically involve catalytic enzymes, which can have non-trivial transport properties, in particular chemotaxis-like directed motion along gradients of substrates and products. Here, we find that taking into account enzyme chemotaxis in models of catalyzed reaction networks can lead to their spatial self-organization in a process similar to biomolecular condensate formation. We develop a general theory for arbitrary reaction networks, and systematically study all closed unimolecular reaction networks involving up to six chemicals. Importantly, we find that network-wide propagation of concentration perturbations can be key to enabling self-organization, in a manner which is highly sensitive on the global network structure.

CPP 18.11 Tue 12:15 BAR/SCHÖ

Spatial organisation of the cell's metabolic power plant via phase separation — •Kathrin S. Laxhuber[1,2] and Frank Jülicher[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck School Matter to Life

Cell metabolism is the power plant that fuels the active processes essential to life. Recent experimental results show that glycolytic enzymes, central to sugar metabolism, phase-separate to form foci under energetic stress and can localise to sites of demand. To understand this phenomenon, we build and study a minimal theoretical model. We show that droplet formation can act as a metabolic switch that enables the system to maintain energetic homeostasis at higher output power. Notably, the metabolic droplets that emerge from this switch can self-organise to colocalise with demand. We discuss the non-equilibrium features and spatial energetic profiles in this system.

CPP 18.12 Tue 12:30 BAR/SCHÖ

Emergent interactions lead to collective frustration in robotic matter — •Onurcan Bektas[1,3], Adolfo Alsina[2,3], and Steffen Rulands[1,3] — [1]Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoSciences, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 München, Germany — [2]GISC, Universidad Rey Juan Carlos, Tulipán, 28933, Móstoles, Spain — [3]Max-Planck-Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany

Current artificial intelligence systems show near-human-level capabilities when deployed in isolation. Systems with intelligent agents are deployed to perform tasks collectively. This raises the question of whether robotic matter, where many learning and intelligent agents interact, shows emergence of collective behaviour. And if so, what kind of phenomena would such systems exhibit? Here, we study a paradigmatic model for robotic matter: a system composed of a large collection of stochastic interacting particles where each particle is endowed with a deep neural network that optimizes its transitions based on the particles' environments. For a 1D model, robotic matter exhibits complex phenomena arising from emergent interactions, including transitions between long-lived learning regimes, the emergence of particle species, and frustration. We also find an abrupt, density-dependent change in the behaviour of particles. Using active matter theory, we show that this phenomenon is a reflection of a phase transition with signatures of criticality. Our model captures key phenomena observed in more complex forms of robotic systems.

CPP 19: Focus Session: Water – from Atmosphere to Space I (joint session CPP/DY)

Water plays a vital role in diverse Earth processes across multiple scales, from atmospheric cycles and aerosol chemistry to geological porous media and nanoscale biological functions of hydrated proteins. Despite its fundamental importance and numerous anomalous properties, such as the diverging heat capacity of supercooled water, pure bulk water remains poorly understood. Key phenomena like evaporation and crystallization are relevant not only on Earth but also in extraterrestrial environments. In Germany, molecular water research is flourishing across prestigious centers, exemplified by the new BlueMat cluster at Hamburg University of Technology, the renewed RESOLV cluster at Ruhr-University Bochum, and the Max Planck Society's expanding Liquid Initiative in Mainz. The 2025 inauguration of the Centre for Molecular Water Science (CMWS) at Hamburg's DESY campus further strengthens a Europe-wide interdisciplinary network, uniting 47 founding members from 12 countries to advance water science across disciplines and methods. Within this focus session the state of molecular water research shall be discussed and interactions between the physical sub-fields shall be fostered.

Organized by Alexander Schlaich, Katrin Amann-Winkel, Mischa Bonn.

Time: Tuesday 9:30–11:00 Location: ZEU/LICH

Topical Talk CPP 19.1 Tue 9:30 ZEU/LICH
Surface adsorption and protonation equilibrium of atmospheric organics at the aqueous surface — •Nønne Prisle — Center for Molecular Water Science, Deutsches Elektronen-Synchrotron DESY, Notkestrasse 85, D-22607 Hamburg, Germany — Institute of Inorganic and Applied Chemistry, University of Hamburg, Martin-Luther-King-Platz 6, D-20146 Hamburg, Germany — Center for Atmospheric Research, University of Oulu, P.O. Box 4500, FI-90014, Oulu, Finland

Atmospheric aerosols comprise a significant fraction of organic species which frequently exhibit both surface activity and Brönsted acidity or basicity in aqueous solutions. The high surface area to bulk volume ratios of nano- and microscopic aerosols and droplets further favor surface-specific states, affecting both bulk-phase and heterogeneous chemistry.

We used X-ray Photoelectron Spectroscopy (XPS) in combination with high-brilliance synchrotron radiation to directly observe the protonation state of atmospheric acids and bases at the surfaces of aqueous aerosol and droplet models. We found that for each acid-base pair, the neutral species is enhanced in the surface, consistent with its higher surface activity, compared to the charged conjugate. This introduces a shift in the protonation equilibrium at the aqueous surface corresponding to an apparent change in pKa of 1-2 pH units, depending on the concentration, acidity, and surface activity of the conjugate acidic and basic species.

CPP 19.2 Tue 10:00 ZEU/LICH
The Effect of pH on the Structure of Model Sea Spray Aerosol Surfaces — •Clara M. Saak, Lars Höhner, and Ellen H.G. Backus — Institute of Physical Chemistry, Faculty of Chemistry, University of Vienna, Währinger Straße 42, 1090 Vienna, Austria

Aerosols play a key role in the global climate due to their ability to scatter and reflect solar radiation and to act as cloud condensation nuclei (CCN), exerting a pronounced cooling influence on the global climate. In particular, the surface availability of ions and organic compounds is known to affect the hygroscopicity of the particle and thereby its ability to act as a CCN [1]. While the surface propensity of individual compounds has been studied widely, much less is known about more complex systems. Here we focus on the impact of bulk pH on the architecture of mixed aqueous interfaces. In atmospheric systems the pH has been shown to range from roughly pH 8 to 2 [2]. Using sum-frequency-generation (SFG) spectroscopy in conjunction with surface tension data we study the surface composition and structure of short and long chain organic acids at different protonation stages, obtained by varying the pH. Using this approach, we find pronounced changes in the structuring of the aqueous sub-surface layers depending on the specific composition and pH, and in the Gibbs free energy of adsorption of the studied organics. Our results show that it is feasible for subtle environmental changes to considerably affect structure and composition of the aqueous interface, which is known to play a key role in aerosol hygroscopicity. [1] Zieger, Nat. Commun. 2017, 8, 15883. [2] Angle, PNAS, 2021, 118, 2, e2018397118

CPP 19.3 Tue 10:15 ZEU/LICH
Crystallization behaviour of nanoparticle suspensions — •Isabell Zick[1,2], Eduard Edel[2], and Katrin Amann-Winkel[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudinger Weg 7, 55128 Mainz, Germany — [2]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

Water is one of the most abundant substances in the world and due to this in close contact with many materials including micro- and nanoplastic particles. Those have been detected not only in sea but also in the atmosphere, where the particles can interact with water and act as cloud condensation nuclei or ice-nucleating particles. Emerging evidence suggests that nanoparticles with increased surface roughness or chemical functionalities may promote heterogeneous ice nucleation through different processes like, e.g., contact- and immersion-freezing. Such a behaviour affects cloud properties with significant implications for Earth*s radiative balance and the hydrological cycle.

We investigate atmospherically relevant nanoparticles dispersed in water to investigate their influence on the ice crystallization. Our experiments include calorimetry (DSC) as well as X-ray diffraction measurements (XRD). Our measurements show that the crystallization temperature depends on the particle size, concentration, and the chemical surface of the particles. Using XRD, we investigate the restructuring of the water molecules during supercooling, observed by a shift in the characteristic main diffraction peak of water and the subsequent crystallization process.

CPP 19.4 Tue 10:30 ZEU/LICH
Laser-Excited X-ray Reflectivity of Aqueous SrCl2 at the Air-Water Interface — •Ali Ashtiani Abdi[1,2], Julia Kobus[1,2], Svenja C. Hövelmann[1,2], Philipp Jordt[1,2], Nicolas Hayen[1,2], Prashant Hitaishi[1,2], Ajay Ajay[1,2], Rabia Qamar[1,2], Otto Lippmann[1,2], Chen Shen[3], Florian Bertram[3], and Bridget M. Murphy[1,2] — [1]IEAP, CAU Kiel University, Kiel, Germany — [2]Ruprecht Haensel Laboratory, DESY, Hamburg, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Understanding aqueous interfaces is essential for describing chemical processes in atmospheric, marine, and geochemical environments. While monovalent salts have been widely studied, the interfacial behavior of divalent ions is less understood, despite their relevance in seawater aerosols and reactive brines. SrCl2 is a representative divalent electrolyte whose interfacial structure may show alteration by laser illumination.

We investigate aqueous SrCl2 solutions at different concentrations using X-ray reflectivity (XRR) at the liquid-air interface. Measurements were performed at the LISA setup at beamline P08, PETRA III (DESY), where controlled laser illumination can be applied directly to the X-ray footprint, following the instrumentation concept of Warias and Hovelmann et al. (J. Synchrotron Rad. 2024). Reflectivity curves were recorded with and without laser exposure. The data demonstrate the suitability of SrCl2 surfaces for laser-assisted XRR and the sensitivity of the method to potential changes in interfacial structure, including indications of near-surface layering.

CPP 19.5 Tue 10:45 ZEU/LICH
Monitoring Uptake, Release and Reaction of Gases at the Liquid-Vapor Interface — •Tillmann Buttersack[1], Shirin Gholami[1], Clemens Richter[1], Daniela Torres-Diaz[1], Bernd

Winter[1], Pavel Jungwirth[2], Stephen Bradforth[3], Markus Ammann[4], Ruth Signorell[5], Ivan Gladich[6], Remi Dupuy[7], Philip Mason[2], and Hendrik Bluhm[1] — [1]Fritz Haber Institute, Max Planck Society, Berlin, GER — [2]IOCB, Czech Academy of Sciences, Prague, CZ — [3]University of Southern California, Los Angeles, USA — [4]Paul Scherrer Institut, Villigen, CH — [5]EZH Zürich, CH — [6]University of Urbino, Urbino, I — [7]Sorbonne Université, Paris, F

Multiphase reactions are omnipresent in nature, industrial applications. The direct observation of reactions at the liquid-vapor interface requires spectroscopic techniques that are surface specific and chemically sensitive to detect low concentrations, e.g., photoelectron spectroscopy (XPS). Furthermore, the sample delivery method must allow sufficient time for an interface reaction to proceed. These complex challenges require individual approaches for each system of interest. One example for a multiphase process is the reaction between liquid alkali metal and water vapor, which is extremely fast. We used a slow droplet train of NaK in a wet atmosphere and observed the formation of golden aqueous solutions with metallic properties with XPS. An example with relevance for atmospheric chemistry is the formation and the release of sulfur dioxide (SO2) from aqueous sulfite solutions due to acidification. We demonstrated that dissolved gases can be detected with XPS even though their concentration is only about 1 mM.

CPP 20: Complex Fluids and Soft Matter (joint session DY/CPP)

Time: Tuesday 9:30–12:45 Location: ZEU/0160

CPP 20.1 Tue 9:30 ZEU/0160

Process-Directed Self-Assembly of Copolymer Blends: Micro- and Macrophase Separation — •Jiayu Xie and Marcus Müller — Institute for Theoretical Physics, Georg August University Göttingen, 37077 Göttingen, Germany

The equilibrium phase behavior of binary diblock copolymer blends involves a complex interplay between microphase and macrophase separation. We investigate blends of linear diblock copolymers, A_1B_1 (cylinder-forming) and A_2B_2 (cylinder- or lamella-forming), using a combination of self-consistent field theory (SCFT) and single-chain-in-mean-field (SCMF) simulations. When the chain-length asymmetry between the A_1B_1 and A_2B_2 copolymers becomes large, the equilibrium phase diagram exhibits a wide macrophase-separation channel. Strikingly, our simulations reveal a strong pathway dependence within this region: rapid quenching yields a spatially homogeneous structure with narrow cylinder-size distributions and strong hexagonal order, whereas gradual annealing promotes local demixing, resulting in bimodal domain sizes and weaker order. We demonstrate that this process-dependent nonequilibrium behavior can be explained by the distinct evolutions of the system state and free-energy landscape of the blends under quenching or annealing. These findings highlight how different processing conditions can direct nanostructure formation in block copolymer blends, and establish a mechanistic link between processing pathway and the final morphology, thus offering insights into rational design of targeted nanostructured materials.

CPP 20.2 Tue 9:45 ZEU/0160

Topological defect engineering enables size and shape control in self- assembly — Lara Koehler[1,3], Markus Eder[2], Vincent Ouzan-Reboul[3], Christoph Karfusehr[2], Andrey Zelenskiy[3], Pierre Ronceray[4], Friedrich Simmel[2], and •Martin Lenz[3] — [1]MIPPKS, Dresden, Germany — [2]TU Munich, Germany — [3]U. Paris-Saclay, Orsay, France — [4]Aix-Marseille-Université, Marseille, France

Equilibrium self-assembly is a powerful way to build nano- and microscale structures out of interacting subunits. The size and shape of such structures must be controlled in many biological and technological functions, posing significant practical challenges as current strategies require multiple subunit types or the precise control of their shape and mechanics. Here we introduce an alternative approach that circumvents these obstacles. Our method uses subunits whose interactions promote crystals, but also favor crystalline defects. We show theoretically that the magnitude of these interactions, which is well controlled in experiments, governs the self-assembly through topological restrictions on the scope of the defects. Using DNA origami, we demonstrate both size and shape control in two-dimensional disk- and fiber-like assemblies. Our basic concept of defect engineering operates well beyond these examples, and provides a broadly applicable framework to control self-assembly.

CPP 20.3 Tue 10:00 ZEU/0160

Soft colloidal monolayers under drying conditions — •Kai Luca Spanheimer[1], Maret Ickler[2], Julian Ringling[3], Nicolas Vogel[2], Matthias Karg[4], and Hartmut Löwen[1] — [1]Insitut für Theoretische Physik II, Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [2]Institute of Interfaces and Particle Technology, Friedrich-Alexander University, Erlangen, Germany — [3]Physikalische Chemie I: Kolloide und Nanooptik Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [4]Institut für Chemie, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany

Langmuir-Blodgett deposition is a well established technique in research and industry. Even though, there still are effects in this process that are not yet explored from a theoretical standpoint. It is usually assumed that the deposited pattern is identical with the one appearing at the water-air interface. In recent experimental studies, strong reorganization during the drying of soft colloidal monolayers has been observed [1]. Capillary forces during drying are known to change nanoscopic structures, sometimes even leading to their destruction. To model these processes we propose a combination of overdamped particle dynamics coupled to dewetting dynamics of an evaporating liquid film. The patterns produced by this model fit those observed in experiment. This theoretical approach allows exploration of the drying dynamics. Thereby we gain new insights into the drying process and makes experimental results produced with Langmuir-Blodgett deposition more reliable.

[1] K. Kuk, et al: Adv. Sci., 11, 2406977 (2024).

CPP 20.4 Tue 10:15 ZEU/0160

Mechanical assessment of microfluidically-generated poroelastic microgel particles — Aude Sagnimorte[1,2], Anke Lindner[2], and •Joshua McGraw[1] — [1]Gulliver-CNRS, ESPCI-PSL, 10 rue Vaquelin, 75005 Paris — [2]PMMH-CNRS, ESPCI-PSL, 10 rue Vaquelin, 75005 Paris

Soft microgels have numerous applications in diverse fields,such as tissue engineering, drug delivery systems, soft robotics, or as model systems for suspensions or colloids. Among these, photopolymerized hydrogels such as poly(ethylene glycol) diacrylate (PEGDA) are commonly used due to their highly tunable mechanical properties. However, proper characterisation of these properties is challenging, in part due to their small scale, on the order of tens of microns, and in particular the lack of assessment of their time-dependent properties. Here we provide a comprehensive mechanical characterisation of individual photopolymerised microgels particles using atomic force microscopy (AFM) for precise local measurements. In particular, we performed indentation-relaxation tests on PEGDA microdisks immersed in water. By varying indentation depth and probe diameter, we changed the contact area and observed relaxation responses which are indicative of poroelastic behaviour. In particular, larger contact areas resulted in longer relaxation times. Our results also show that increasing the amount of solvent increased the relaxation time. Our collected results are consistent with a simple, Herzian poroelastic model giving good agreement with both the approach and relaxation phases of the experiments.

CPP 20.5 Tue 10:30 ZEU/0160

Nonlinear Viscoelastic Response and Stress Shielding in Driven Bistable Spring Chains — •Sven Pattloch[1,2] and Joachim Dzubiella[1,2] — [1]Applied Theoretical Physics-Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, D-79104 Freiburg, Germany. — [2]Cluster of Excellence livMatS@FIT-Freiburg Center for Interactive Materials and Bioinspired Technologies, Albert-Ludwigs-Universität Freiburg, D-79110 Freiburg, Germany

Bistable micromodules are a promising route to design adaptive mechanical metamaterials with tunable viscoelastic response. Here, a driven one-dimensional chain of bistable springs is studied in which both the mechanical deformation and the internal excitation states evolve dynamically under time-dependent forcing. Their coupling produces rich nonlinear viscoelastic behaviour, including frequency-dependent susceptibilities, delayed deformation, and pronounced hysteresis in cyclic loading.

Using analytical linear response theory complemented by numerical simulations, the model quantifies how microscopic parameters and driving protocols control effective stiffness, loss, and phase lags. A key result is a strong attenuation ('shielding') of stress propagation along the chain that is already present for monostable springs but is markedly amplified by excitation switching in bistable modules. These findings provide simple design principles for tailoring nonlinear viscoelasticity, hysteresis, and stress shielding in driven soft matter and mechanical metamaterial systems.

CPP 20.6 Tue 10:45 ZEU/0160

Euler buckling on curved surfaces — •Shiheng Zhao[1,2,3] and Pierre A. Haas[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Max Planck Institute of Molecular Cell Biology and Genetics — [3]Center for Systems Biology Dresden

Nearly three hundred years ago, Euler showed that an inextensible straight elastic line in the plane buckles under compression when the compressive force F reaches a critical value $F_* > 0$. But how does such an elastic line buckle within a general curved surface? Here [1], we reveal that the classical instability changes fundamentally: By weakly nonlinear analysis of the buckling of an asymptotically short elastic line, we show that the critical force for the lowest buckling mode is $F_* = 0$ and discover a new bifurcation structure in which the modes of classical Euler buckling split into pairs. For long elastic lines, we numerically find an additional bifurcation by which the second of these new modes becomes the lowest mode and show that, at sufficiently large F, they undergo discontinuous snap-through to higher end-to-end compression. We explain these bifurcations in terms of the general unfolding of a pitchfork. This constitutes the foundations for a class of mechanical instabilities within curved surfaces from which, for example, biological shape emerges in development.

[1] S. Zhao and P. A. Haas, Phys. Rev. Lett. (in press)

15 min. break

CPP 20.7 Tue 11:15 ZEU/0160

Linking molecular dynamics and experimental FORCs in multicore magnetic nanoparticles — Ekaterina Novak[1], •Malika Khelfallah[2], Andrey Kuznetsov[3], Deniz Mostarac[4], Claire Carvallo[2], Amélie Juhin[2], and Sofia Kantorovich[3] — [1]Ekaterinburg, Russia — [2]Sorbonne Université, Paris, France — [3]University of Vienna, Vienna, Austria — [4]University of Edinburgh, Edinburgh, United Kingdom

Multicore magnetic nanoparticles - clusters of several magnetic grains embedded in a nonmagnetic matrix - exhibit collective behaviour distinct from single-core particles and are promising candidates fro drug targeting and magnetic hyperthermia. Their magnetic cores possess finite anisotropy, and the multicore assemblies range from near-spherical to elongated ellipsoids, features that strongly affect their response to external fields. To study these effects, we use molecular dynamics simulations [1] to model internal structure, anisotropy distribution, and collective switching. As a key diagnostic, we employ First Order Reversal Curves [2], which experimentalists routinely measure for immobilised multicore particles, enabling direct comparison between simulations and experiments. FORC diagrams reveal coercivity distributions and magnetic interactions between grains, offering detailed insight into interaction mechanisms and domain processes.

The work was financially supported by the RSF grant No. 25-22-00762.

[1] R. Weeber et al. (2024), Comprehensive Computational Chemistry, 3, 578-601. [2] C. R. Pike et al., J. Appl. Phys., 1999, 85, 6660

CPP 20.8 Tue 11:30 ZEU/0160

Hydrodynamics substantially affects induced structure formation in magnetic fluids — •Henning Reinken and Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg, Germany

Magnetorheological fluids consist of micrometer-sized magnetic particles suspended in a carrier liquid [1]. Sufficiently strong external magnetic fields lead to the formation of string-like particle aggregates, which results in complex magnetorheological behavior. This mechanism can further be used in the production of magnetic elastomers during the polymerization process when the carrier medium is still fluid and particulate structure formation still possible [2]. Using numerical simulations that spatially resolve both fluid flows and magnetization, we demonstrate that hydrodynamic interactions play a substantial role during structure formation. Hydrodynamics supports the emergence of string-like aggregates, while magnetic interactions align them. Considering besides this fundamental insight the enormous technical importance and potential of magnetic fluids, our results are substantial also from an application perspective.

We acknowledge support by the German Research Foundation DFG through Research Unit FOR 5599 on structured magnetic elastomers.

[1] S. Odenbach, Arch. Appl. Mech. **86**, 269 (2016).

[2] D. Günther, D. Yu Borin, S. Günther, S. Odenbach, Smart Mater. Struct. **21**, 015005 (2012).

CPP 20.9 Tue 11:45 ZEU/0160

Near-surface colloidal dynamics in jammed and slipping microgel suspensions — •Masoodah Gunny[1], Frédérick Caetano[2], Matilde Bureau[2], Alexandre Vilquin[1], Marie Le Merrer[2], Catherine Barentin[2], and Joshua McGraw[1] — [1]Gulliver - CNRS, ESPCI-PSL 10 Rue Vauquelin 75005 Paris, France — [2]ILM - CNRS, Claude Bernard University, 16 Enrico Fermi 69100 Villeurbanne, France

Jammed suspensions of soft microgel particles exhibit wall slip along smooth boundaries. The direct observation of dynamics within a supposed depletion layer near the wall were difficult to achieve as a result of the layers' supposed sub-micrometric dimensions. We use total internal reflection fluorescence microscopy (TIRFM) to observe colloidal-particle dynamics near the interface between glass and microgel suspensions. Remarkably, microgel suspensions display nanoscale velocity profiles with a slope rupture; particle velocity increases with distance near the wall, and tends to a constant beyond a distance which is characteristic of the ones predicted previously. Beyond velocimetry, we also study the statistical particle altitude distributions near the wall in TIRFM measurements. These distributions are strongly pressure dependent, with nanoparticles more likely found near the solid/liquid interface when the fluid is transported faster near the wall. This high-velocity particle enrichment, not seen for the Newtonian case, is consistent with the development of a depletion layer under such conditions. Taken together, our observations give strong support for the existence of a depletion layer being responsible for wall slip.

CPP 20.10 Tue 12:00 ZEU/0160

Random close packing as a conserved directed percolation transition — •Thomas Axmann and Michael Schmiedeberg — Theoretical Physics: Lab for Emergent Phenomena, Soft Matter Theory Group, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

In studying quenches in soft sphere systems O'Hern et al. related the onset of overlaps to isostaticity [1], and consequently to the random close packing scenario. The conditions that lead to the avoidance of overlaps between spheres can be studied with the random organization model [2], which was initially introduced to investigate self organization in sheared colloids. Modifications of this model, which dynamically reduce interparticle overlaps, were used to characterize the random close packing problem as the critical point of a dynamic absorbing state transition in the $d+1$ dimensional conserved directed percolation universality [3,4].

We aim to deepen the understanding of this connection by demonstrating that the configuration change at each time step can be chosen with a fully deterministic strategy while retaining the features of the transition. We clarify difficulties in the treatment of percolating clusters and find that the median overlap depth proves to be a more useful order parameter.

[1] O'Hern et al. PRE 68 (2003)

[2] Corté et al. Nat. Phys. 4 (2008)

[3] Milz et al. PRE 88 (2013)

[4] Wilken et al. PRE 128 (2021)

CPP 20.11 Tue 12:15 ZEU/0160

Rescaled mode-coupling scheme for dynamics in binary mixtures of highly charged colloids — •Daniel Weidig and Joachim Wagner — University of Rostock, Rostock, Germany

We investigate dynamic processes in binary mixtures of highly charged colloidal particles by means of Brownian dynamics and multi-component mode-coupling theory (MCT). As input for MCT, thermodynamically consistent, static structure factors from integral equations

with Rogers-Young closure are used which are in quantitative agreement to Fourier transforms of static pair correlation functions resulting from simulations.
MCT based on partial structure factors in many-particle systems predicts dynamic properties such as long-time self-diffusion coefficients in qualitative agreement to simulation trajectories. Using instead structure factors from systems with slightly reduced number of effective charges as input, a quantitative agreement of MCT with simulations is achieved. In mixtures of identically charged particles with different short-time mobilities, this rescaled MCT scheme accurately predicts coupling effects in long-time dynamics observed in Brownian dynamics simulations.

CPP 20.12 Tue 12:30 ZEU/0160

Electric double layers - the software package capDFT — Fabienne Dressler and •Andreas Härtel — Institute of Physics, University of Freiburg

Electric Double Layers are used to store electric energy, they can be utilized to harvest energy from waste heat or steps in concentrations, and they stabilize colloidal systems. In all cases, mobile ions arrange themselves to screen surface charges, resulting in sometimes densely packed regions of microscopic particles far from bulk states that dominate the macroscopic physical properties of the system. Modeling these complex systems has theoretical and numerical limitations, but good although expensive solutions exist. We present an open-source software package to treat the described modeling utilizing classical density functional theory [1]. The package has been used successfully in studies of underscreening [2] and allows to go beyond the standard mean-field approximation of primitive models [3]. We will demonstrate the package by discussing an example, where we study capacities of structured electrodes.

[1] https://github.com/andreashaertel/capdft
[2] Anomalous Underscreening in the Restricted Primitive Model. A. Härtel, M. Bültmann, and F. Coupette. Phys. Rev. Lett. 130, 108202 (2023)
[3] The primitive model in classical density functional theory: beyond the standard mean-field approximation. M. Bültmann and A. Härtel. J. Phys. Condens. Matter 34, 235101 (2022)

CPP 21: French-German Session: Simulation Methods and Modeling of Soft Matter III

Time: Tuesday 9:30–11:15 Location: ZEU/0255

Invited Talk CPP 21.1 Tue 9:30 ZEU/0255

Molecular modelling of gas solubility and free volume trends in Si-functionalized ionic liquids — •Kateryna Goloviznina[1,2], Eduards Bakis[3], Inês C. M. Vaz[2,4], Agilio Padua[2], and Margarida Costa Gomes[2] — [1]ICSM, University of Montpellier, CEA, CNRS, ENSCM, 30207 Bagnols-sur-Ceze, France — [2]Laboratoire de Chimie, ENS de Lyon and CNRS, 46 allée d'Italie, 69364 Lyon, France. — [3]Faculty of Chemistry, University of Latvia, Jelgavas 1, Riga, LV-1004, Latvia. — [4]CICECO, Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal

Molecular dynamics (MD) simulation is a powerful technique that provides insight into the nanoscale structure and transport properties of liquids in bulk and at interfaces, explaining experimentally observed phenomena and contributing to the rational design. In the present work, we explored Si-functionalized imidazolium-based ionic liquids—low-density, low-viscosity systems—that are promising for gas capture and separation due to their enhanced free volume. [1] Using classical MD simulations with the CL&Pol polarizable force field, [2] we proposed a way to estimate free-volume trends and solubilities of simple gases (e.g., argon) without the need to perform costly experiments. The work was further extended to unsaturated C_2 hydrocarbons, for which we rationalized solubility trends via local structural analysis and estimated the contributions of van der Waals, electrostatic, and polarization terms to the solvation free energy.
[1] E. Bakis et al. Chem. Sci. 2022, 23, 9062.
[2] Goloviznina et al. J. Chem. Theory Comput. 2019, 15, 5858.

CPP 21.2 Tue 10:00 ZEU/0255

Classical DFT compared to AFM measurement of structural forces from confined electrolyte containing charged nanoparticles — •Simone Riva[1], Michael Ludwig[2], Regine von Kltizing[2], and Ofer Manor[1] — [1]Technion, Haifa, Israel — [2]Technische Universität Darmstadt, Darmstadt, Germany

We use classical density functional theory (DFT) to model colloidal-probe atomic force microscopy (AFM) force curves across an aqueous electrolyte containing charged solid nanoparticles. The charged AFM probe and substrate interact through a suspension of silica nanoparticles. The probe experiences oscillatory forces driven by the structuring of the charged nanoparticles, which can enhance the stability of the film. Structural forces are characterized by an alternation of repulsion due to steric and electrostatic nanoparticle interactions, and depletion attraction. We present a self-consistent theory of oscillatory forces in ionic systems. Moreover, we compare different DFT approaches and validate them against AFM measurements, to develop a theory that best fits the rich physics of experiments. We calculate structural and EDL forces by minimizing dedicated functionals. We adopt two types of weighted density functionals, disclosing their applicability in different concentration conditions. We propose a way to include electrostatic interactions between nanoparticles in an effective hard-sphere functional. We further confirm a general scaling law of the oscillation wavelength observed in experiments and connect it to nanoparticle packing structures. The theory agrees well with measurement in the absence of fitting parameters. Riva et al., JCIS 2026, 702, 138901.

CPP 21.3 Tue 10:15 ZEU/0255

Sc-cDFT: A Single-Chain Simulation Framework with Classical Density Functional Theory for Polymers — •Raju Lunkad[1], Alejandro Gallegos[2], Jianzhong Wu[3], and Marcus Müller[1] — [1]Institute for Theoretical Physics, Georg-August University, 37077 Göttingen, Germany — [2]Department of Chemical and Materials Engineering, New Mexico State University, Las Cruces, New Mexico 88001, United State of America — [3]Department of Chemical and Environmental Engineering, University of California, Riverside, CA, United States of America

We present Sc-cDFT, a combination of Single-Chain Simulation with classical Density-Functional Theory (cDFT), for modeling polymer solutions and brushes. In this approach, intramolecular correlations are explicitly treated using Monte-Carlo (MC) simulations, while intermolecular correlations are extracted from cDFT. In this way, we capture structural properties and thermodynamics of multi-chain systems while providing a segment-level description of the dynamic behavior. Importantly, this framework substantially reduces computational cost, enabling the simulation of significantly longer polymer chains that are often inaccessible to fully explicit particle-based simulations. We validate the Sc-cDFT framework for hard-sphere polymer solutions and brushes by comparing polymer configurations and the segmental density profiles with fully explicit particle-based simulations, showing quantitative agreement.

CPP 21.4 Tue 10:30 ZEU/0255

Adsorption Thermodynamics and Kinetics of Complex Fluids: Physical Modeling of Surface Saturation, Reservoir Depletion, Lateral Interactions, and Collective Effects — •Nada Ben Amor[1,2], Daniela Bauer[1], Benjamin Braconnier[1], and Benoit Coasne[2,3] — [1]IFP Energies nouvelles, 92852 Rueil-Malmaison, France — [2]Université Grenoble Alpes, CNRS, LIPhy, F-38000 Grenoble, France — [3]Institut Laue Langevin, F-38042 Grenoble, France

Adsorption at solid surfaces is considered a promising technique to capture and remove emerging pollutants such as PFAS from water. However, a major gap in the literature remains in modeling complex adsorption mechanisms. Three key factors were identified for modeling adsorption thermodynamics and kinetics: surface saturation, reservoir depletion, and lateral interactions. While the first is captured by the celebrated Langmuir model, reservoir depletion, which is crucial for assessing adsorption in batch and dynamic experiments, is often neglected in classical kinetic models. Lateral interactions are also important for pollutants like PFAS as they undergo cooperative adsorption. A 2D lattice gas model with two- and three-body lateral interactions is solved using mean-field and quasi-chemical approximations. The resulting thermodynamics lead to a phase diagram predicting complex adsorption isotherms in agreement with available experiments as well as a first-order dilute to dense phase transition. A mixed-order kinetic model including all three factors is proposed and both thermodynamic and kinetic models are successfully applied to experimental data.

CPP 21.5 Tue 10:45 ZEU/0255

Molecular Dynamics Insights into Thermodynamic and Structural Properties of Water Adsorbed Poly(Heptazine Imide) Zeolites — •Youssef Mabrouk[1], Akshey Suresh[2], Yizak Tzegazab[2], Lingli Ni[2], Martin Oschatz[2], Alexander Croy[1], and Stefanie Gräfe[1] — [1]Friedrich Schiller University of Jena, Insitute of Physical Chemistry, Lessingstraße 4, 07743 Jena, Germany — [2]Friedrich Schiller University of Jena, Institute for Technical Chemistry and Environmental Chemistry, Philosophenweg 7a, 7743 Jena, Germany

The recently reported reversible water adsorption of porous layered carbon nitrogen frameworks suggests their high potential as functional materials for energy storage and conversion applications specifically in view of the controlled crystallinity and polarity and water binding motifs these frameworks offer. Based on molecular dynamics simulations of pressure-controlled solid/gas equilibrium isotherms, the framework structure-dependent adsorption of water in poly(heptazine imides) is here investigated. Using minimal motifs of heptazine sheets in pressure-controlled water vapor environments, the load-dependent transition from monomolecular to condensation-limited adsorption is furthermore investigated. The hydrophilicity characterized by the isotherms agree with physiosorption experiments. The layer planarity and pore geometry-dependent crystallinity characterized by the structure factor and normal modes agree with x-ray diffraction and infrared spectroscopy experiments. Overall, our results contribute to identifying the relevance of each structural motif to adsorption.

CPP 21.6 Tue 11:00 ZEU/0255

Insights into phenylalanine self-assembly and its modulation by nucleotides from molecular dynamics simulations. — •Mattia Borriello — Ruhr-Universität Bochum

Phenylalanine (Phe) can aggregate in water into various fibrillar structures, which is relevant to diseases like phenylketonuria. The precise molecular structure of these aggregates is still unknown, and although they dissolve in the presence of nucleotides such as ATP, the mechanism behind this disassembly remains unclear. We use molecular dynamics simulations to gain new insights on Phe cluster structure, understand which interactions drive this process and how nucleotides can modulate it.

Parallel tempering simulations of Phe in water in zwitterionic form have been performed varying concentration and temperature. Analysis of the trajectories revealed a strong tendency to aggregate in two ordered structures. One is characterized by a tubular shape, while the other by an alternating motif. Cluster stabilization is mainly electrostatic for smaller aggregates, while apolar interactions become significant as the size of the clusters grows.

The same computational approach has been extended to systems containing Phe and NaCl or different nucleotides, such as ATP, ADP and AMP. While NaCl showed a limited influence on aggregation, nucleotides can inhibit cluster formation and disrupt pre-existing aggregates. Our findings provide molecular-level insight into both the structural organization of Phe assemblies and into the mechanisms through which nucleotides modulate their stability.

CPP 22: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics I

Time: Tuesday 9:30–11:15 Location: ZEU/0260

Invited Talk CPP 22.1 Tue 9:30 ZEU/0260

From Solution to Thin Films: Structure Formation Pathways in Organic Photovoltaic Films — •Eva M. Herzig — Dynamik- und Strukturbildung - Herzig Group, University of Bayreuth, Germany

The performance of organic solar cells is governed by a delicate interplay between molecular packing, phase separation, and mesoscale connectivity in donor-acceptor blends. It is therefore highly desirable to control structure formation; however, this remains a non-trivial task. Several factors contribute simultaneously: the initial aggregation state in solution [1,2], the rapid structure formation during solution processing [2], and subsequent temperature- or solvent-annealing steps [3,4]. In this talk, I will discuss and illustrate with selected examples at which of these stages the final thin-film morphology can be controlled.

Using time-resolved and multimodal characterization methods, including grazing-incidence X-ray scattering and optical spectroscopy, we resolve the evolving structures during and after film deposition. These measurements reveal how subtle variations in processing conditions translate into distinct nanoscale morphologies.

[1] F. Eller & E. M. Herzig, J. Phys. Chem. A 2024, DOI: 10.1021/acs.jpca.4c04902

[2] F. Eller, R. Hildner, R. W. A. Havenith & E. M. Herzig, Small 2023, DOI: 10.1002/smll.202207537

[3] F. Eller, C. R. McNeill & E. M. Herzig, Adv. Energy Mater. 2024, DOI: 10.1002/aenm.202304455

[4] M. Kuhn, X. Huang, M. Gebert, L. Thomsen, C. R. McNeill & E. M. Herzig, Adv. Funct. Mater. 2025, DOI: 10.1002/adfm.202509532

CPP 22.2 Tue 10:00 ZEU/0260

DBTTF:HATCN Cocrystals – experimental details on influence of crystal solvents on crystal structure and on charge transfer — •Andreas Opitz[1], Ana M. Valencia[2], Lisa Schraut-May[3], Marie Siegert[3], Sebastian Hammer[3], Beatrice Cula[4], Alexandra Friedrich[5], Holger Helten[5], Jens Pflaum[3], and Caterina Cochi[6] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Institute of Physics, Carl-von-Ossietzky Universität Oldenburg — [3]Experimental Physics VI, Julius-Maximilians-Universität Würzburg — [4]Department of Chemistry, Humboldt-Universität zu Berlin — [5]Institute of Inorganic Chemistry & Institute for Sustainable Chemistry and Catalysis with Boron, Julius-Maximilians-Universität Würzburg — [6]Institute of Condensed Matter Theory and Optics, Friedrich-Schiller-Universität Jena

Donor-acceptor (D:A) cocrystals offer a promising platform for next-generation optoelectronic applications, but the impact of residual solvent molecules on their properties remains an open question. We investigate six novel D:A cocrystals of dibenzotetrathiafulvalene (DBTTF) and 1,4,5,8,9,11-hexaazatriphenylenehexacarbonitrile (HATCN), prepared via solvent evaporation, yielding 1:1 molar D:A ratios with solvent molecules in the structure, and horizontal vapor deposition, resulting in solvent-free 3:2 cocrystals. Optical properties of these materials are largely unaffected by solvent inclusion. The vibrational energy of the cyano mode depends on the dipole moment of the incorporated solvent molecules, but the degree of charge transfer is consistent across all analyzed cocrystals.

CPP 22.3 Tue 10:15 ZEU/0260

Reassessing Mobility Imbalance in Organic Photodetectors for High-Speed Applications — •Felix Hergenhan, Tianyi Zhang, Karl Leo, and Johannes Benduhn — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden

Organic photodetectors (OPDs) are emerging candidates for diverse optoelectronic applications, yet their use in high-speed technologies such as optical communication remains largely believed to be restricted by low effective charge carrier mobilities. To address this challenge, we investigated how the transient behavior of OPDs depends on the mobilities of the respective charge carriers. This relationship is examined through drift-diffusion simulations and experiments across various material systems, under varied bias and illumination conditions. We show, contrary to common assumptions, that obtaining only one fast charge carrier mobility is sufficient to achieve high response speed. Likewise, in systems with pronounced mobility imbalance, the slower carriers do not necessarily govern the maximum operation speed of the device. Leveraging these insights, we demonstrate an OPD tailored for optical communication that achieves data transmission rates up to 170 Mbps, representing one of the highest reported transmission rates for organic-based optical communication systems. These findings establish a refined design framework for ultrafast OPDs, providing guidance on material selection, device design, and operation regimes.

CPP 22.4 Tue 10:30 ZEU/0260

Rational Design of Donor-Acceptor Oligomers for Enhanced Charge Separation — •Jannik Theile[1], Michele Guerrini[2], Surender Kumar[2], and Caterina Cocchi[2] — [1]Physics Department and Center for Nanoscale Dynamics, Carl von Ossietzky Universität Oldenburg, Germany — [2]Physics Department for Solid-State Physics and Optics, Friedrich-Schiller Universität Jena, Germany

Intramolecular charge transfer (ICT) in donor-acceptor (D-A) oligomers is central to organic optoelectronics, yet symmetric D-A-D and A-D-A systems often suffer from delocalized frontier molecular orbitals (FMOs) that hinder efficient photoinduced charge separation. To address this, we present a first-principles study based on (time-dependent) density functional theory of 22 dithieno[3,2-b:2',3'-d]pyrrole oligomers, exploring the interplay between structural asymmetry and site-selective fluorination. Donor fluorination widens the electronic gap, while acceptor fluorination enhances charge imbalance and promotes confinement and spatial segregation of FMOs onto distinct molecular segments. The resulting optical properties reveal asymmetric, acceptor-fluorinated systems as optimal for ICT due to strong charge-transfer excitations with large oscillator strengths in the visible region. This work establishes rational design rules for conjugated D-A oligomers, showing that combining asymmetry with targeted halogenation is key to achieving robust, directional ICT and enabling high-performance organic semiconductors.

CPP 22.5 Tue 10:45 ZEU/0260

Substituted Benzo[*b*]fluorenes as Emitters for OLED With Tunable Electroluminescence in the Full Visible Range — •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 emitting molecules continues, especially in the blue range. Substituted benzo[*b*]fluorenes (BF) show high stability of photoluminescence in solution over months. By exchanging the substitutional pattern, we show that this group of molecules allows for preparation of OLED with tunable emission bands in the full range of the visible spectrum. Thin films of BF can be prepared by solution-based methods or physical vapor deposition, allowing for easy integration into different layer stacks. Photoluminescence spectroscopy of showcase BFs revealed a multi-band emission that is found in line with electroluminescence spectra of the corresponding devices. Contact formation at relevant device interfaces was studied by in-situ Kelvin-probe force microscopy and gave insight into details of film growth and alignment of transport levels. Based on these findings we demonstrate working OLED devices with intense blue or red emission, respectively.

CPP 22.6 Tue 11:00 ZEU/0260

Electrically switchable chiroptical responses in organic ferroelectric thin films — •Lorenz Friedrich Meier[1], Sophia Klubertz[1], Victor Rodriguez[2], Miguel García-Iglesias[2], David González-Rodríguez[3], and Martijn Kemerink[1] — [1]Heidelberg University, Germany — [2]Universidad de Cantabria, Spain — [3]Universidad Autónoma de Madrid, Spain

Organic ferroelectrics potentially allow to introduce switchable polarization into an easily processable material, enabling their integration into next-generation electronic devices. We investigate a liquid-crystalline organic ferroelectric that additionally can exhibit electrically controlled chiroptical responses, relevant for optical data storage, photonic components, and chiroptical sensing. We investigate thin films of trialkylbenzene-1,3,5-tricarboxamide (BTA). These molecules self-assemble into supramolecular columns by forming a triple helix of dipoles connected via hydrogen bonds. By incorporating chirally-biased sidechains, the handedness of the supramolecular helix can be defined. We experimentally show ferroelectric behavior in both in-plane and out-of-plane geometries by double wave and CV measurements. We demonstrate how the unpractically high coercive fields for pure chiral BTA can be reduced by mixing with achiral BTA. Previous simulations show that the energetically preferred mechanism of polarization reversal of a supramolecular column will simultaneously change its chirality. Thus, an electrically switchable chirality is possible. We present an experimental investigation of this mechanism, discussing the challenges including the need for dipole pre-alignment.

CPP 23: Focus Session: Water – from Atmosphere to Space II (joint session CPP/DY)

Time: Tuesday 11:15–12:45 Location: ZEU/LICH

CPP 23.1 Tue 11:15 ZEU/LICH

Microscopic diffusion and reactivity in aqueous solutions: photogenerated nascent halogen atoms, solvated electrons and subsequent dihalide formation — •Zhangatay Nurekeyev[1,2], Hyein Hwang[1,2], Fernando Rodriguez Diaz[1], Mei Bai[3], Michael Thorwart[3], Michaela Schäfer[4], Carmen Herrmann[4], and Christian Bressler[1,2,5] — [1]Inst. of Exp. Physics, Universität Hamburg — [2]The Hamburg Centre of Ultrafast Imaging (CUI) — [3]I. Inst. of Theor. Physics, Universität Hamburg — [4]Dept of Chemistry, Universität Hamburg — [5]European XFEL, Schenefeld

The solvent plays an important role in the assembly, stability and reactivity of (bio)chemical molecules. Small changes of the caging solvent can alter the reaction outcome, but little is known about the atomic-scale solvation shell dynamics. Our approach utilizes aqueous mono-atomic halide solutes, which are transformed into nascent neutral halogen atoms upon femtosecond optical excitation together with a separated solvated electron. Combining X-ray absorption with transient optical absorption spectroscopies we monitor the subsequent diffusion-driven atom-electron recombination, each focusing on the halogen atom and on the solvated electron, respectively. We also monitor the appearance of dihalides on the tens of picosecond time scale. Using all x-ray and laser observables we deliver a new picture of the ensuing dynamics, for which the existence of the long-lived (X:e) contact pair is not required. Next steps aim to trace more complex guest-host scenarios towards functional proteins in solution.

CPP 23.2 Tue 11:30 ZEU/LICH

Surface Propensity of Halide Ions in Water: New Evidence from LJ-XPS — •Daniela Torres-Díaz[1], Shirin Golami[1], Tillmann Buttersack[1], Qi Zhou[1], Rémi Dupuy[2], Bernd Winter[1], Chistophe Nicolas[3], and Hendrik Bluhm[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Laboratoire de Chimie Physique - Matière et Rayonnement (Sorbonne Université, CNRS), Paris, France — [3]Synchrotron SOLEIL, Saint-Aubin, France

The surface propensity of halide ions in water is still a matter of debate. While the famous Onsager&Samaras model indicates that charged species should avoid the interface, more recent Molecular Dynamics simulations that take into account the polarizability of the ions indicate notably that iodide and bromide prefer the interface while chloride and fluoride avoid it. Different models, however, differ in how strong this effect is, while experimental studies have reported contradictory results. Here I will discuss recent results obtained using Liquid-Jet X-Ray Photoemission Spectroscopy on water interfaces for potassium halide solutions. In particular, the measurement of the photoelectron angular distributions allow for a higher spatial resolution than classic XPS measurements.

CPP 23.3 Tue 11:45 ZEU/LICH

Ion Correlations Drive Collective Adsorption of Hydronium Ions at the Air-Electrolyte Interface — •Elena Köhler Ruiz, Maximilian Becker, Louis Lehmann, and Roland Netz — Fachbereich Physik, Freie Universität Berlin, Germany

Acids exhibit distinct interfacial behavior at the air-water interface compared to simple monoatomic salts. While monoatomic ions are largely repelled from the interface, hydronium ions preferentially reside at the interface due to formation of an interfacial hydrogen-bond network. To investigate these contrasting behaviors, we perform molecular-dynamics simulations with thermodynamically optimized force fields, analyzing ionic distributions at the interface as well as resulting surface tensions and potentials. The simulated surface potentials reproduce the concentration-dependent trends observed in SFG experiments: At high concentrations, interfacial hydronium promotes co-adsorption of counterions, which results in a decrease of the surface potential with rising concentration, consistent with experimental observations. These findings highlight the critical role of ion-ion correlations at interfaces, which are not accounted for by modified Poisson-Boltzmann models.

CPP 23.4 Tue 12:00 ZEU/LICH

Calcium-amino acid complexation in water probed by Intermolecular Coulombic Decay — •Michele Pugini, Nicolas Velasquez, Harmanjot Kaur, Florian Trinter, Qi Zhou, Lukas Tomaník, Uwe Hergenhahn, and Bernd Winter — Fritz-Haber-Institut, Berlin

The Ca2+ ion is the most abundant metal ion in the human body, playing essential roles in numerous biological processes, many of which involve interactions with proteins. Gaining molecular-level insight into the nature of the interaction between Ca2+ ions and solvated amino acids is therefore crucial for understanding calcium's biological function. Intermolecular Coulombic decay (ICD), a non-local autoionization process, offers unique sensitivity to the local chemical environment and can selectively probe interactions within the first solvation shell of solvated Ca2+ ions.

Here, we demonstrate the sensitivity of resonant ICD3 to the chemical composition of the solvation shell, enabling the identification of Ca2+ associations with specific amino acids. Our model system is the amino acid proline. The interaction, if present, is revealed via the ICD electrons resulting from the ionization of the biomolecule upon the 2p to 3d excitation of Ca2+.

Our results unequivocally identify Ca2+-proline interactions, indicating substitution of water molecules in the ion's coordination shell by proline. These findings establish ICD as a sensitive probe of metal-biomolecule interactions and highlight its potential as a powerful spectroscopic tool for investigating biomolecular structure in solution.

CPP 23.5 Tue 12:15 ZEU/LICH

Distinguishing cavity and non-cavity solvation structures of the hydrated electron — •Sy Dat Ho and Benjamin Philipp Fingerhut — Department of Chemistry and Centre for NanoScience, Ludwig-Maximilians-Universität München, 81377 München, Germany

Solvated electrons in water are prototypical low-dimensional quantum systems that are coupled to a fluctuating, many-body environment. However, their hydration structure is still a matter of debate, with both cavity and non-cavity models having been suggested. First-principles molecular dynamics simulations are performed of excess-electron localization in liquid water, using hybrid-meta-GGA and hybrid-GGA density functionals that accurately reproduce bulk water structure. Perturbations to the local hydrogen bond structure of water due to interaction with the excess charge are identified, giving rise to specific signatures in transient radial distribution functions. These patterns are then compared with preliminary liquid-phase MeV-UED data obtained during an early science campaign at SLAC. In order to distinguish the structural changes induced by excess electrons in the diffraction patterns, long-time simulations at an unprecedented level of theory are required in order to minimise statistical noise. Our results clarify the coupling of hydrated electrons to solvent fluctuations and provide microscopic insight into polaron formation in disordered condensed phases.

CPP 23.6 Tue 12:30 ZEU/LICH

Mesoscopic Structures in Water/HFIP based Electrolytes — •Sophie Zeilinger[1,2] and Markus Mezger[1] — [1]Center for Nano Structure Research, Faculty of Physics, University of Vienna, AT-1090 Vienna — [2]Institute of Physical Chemistry, Faculty of Chemistry, University of Vienna, AT-1090 Vienna

Previous studies have shown that binary water/hexafluoroisopropanol (HFIP) mixtures exhibit nanoscale heterogeneties that strongly affect properties such as reaction rates. The complex hydrogen bonding network of the binary mixture together with the amphiphilic character of the HFIP molecule provides a sensitive environment in which subtle changes in interactions can generate nanoscale heterogeneties. Here, we study the structure formation in water/HFIP under the influence of hydrophilic and hydrophobic ions by Small Angle X-Ray Scattering (SAXS). Depending on water content, pH, salt concentration and temperature we observe monotonous and oscillatory density correlations with structural parameter on the nanometer length scale. These structures are explained by the coupling of coulombic interactions between charged hydrophilic and hydrophobic ions vs. local fluctuations in water/HFIP concentrations.

CPP 24: French-German Session: Simulation Methods and Modeling of Soft Matter IV

Time: Tuesday 11:30–12:45 Location: ZEU/0255

CPP 24.1 Tue 11:30 ZEU/0255

Systematic coarse-graining with density dependent potential: Application to small organic molecules, multicomponent mixtures and polymers — •Sayan Dutta[1,2,3], Maria C. Lesniewski[4], W. G. Noid[4], Denis Andrienko[5], and Arash Nikoubashman[2,3] — [1]Leibniz-Institut für Polymerforschung — [2]Technische Universität Dresden — [3]Johannes Gutenberg-Universität Mainz — [4]Pennsylvania State University, University Park, PA, USA — [5]Max-Planck Institut für Polymerforschung Mainz

Conventional coarse-graining (CG) approaches approximate the underlying many body interactions through effective pair potentials. Although this strategy works well for reproducing structural and thermodynamic properties in bulk systems, it often fails in heterogeneous systems, such as droplets or films, due to the inherently strong density fluctuations in those systems. To address this issue, we incorporated local-density-dependent potentials (LDPs) that treat these many-body contributions explicitly within a mean-field formalism. We develop a CG force-field framework that integrates LDPs, enabling accurate simulation of conjugated organic molecules, organic liquid mixtures, and polymeric systems. This approach provides a more accurate description of thermodynamic and interfacial properties of these systems. Further, it facilitates the establishment of structure-function description that helps in rational designing of functional materials.

CPP 24.2 Tue 11:45 ZEU/0255

A data-driven decoupled multiscale scheme for anisotropic finite strain magneto-elasticity — •Heinrich T. Roth, Philipp Gebhart, Karl A. Kalina, Thomas Wallmersperger, and Markus Kästner — TU Dresden, Dresden, Germany

Structured magnetorheological elastomers (MREs) are composite materials exhibiting magneto-mechanical coupling effects, such as the magnetostrictive and magnetorheological effect. They consist of magnetizable particles arranged in chain-like structures within a soft elastomer matrix. As explicitly resolving their microstructure in real-world samples is infeasible, a multiscale modeling approach is required.

In this work, we present a framework for the macroscale modeling of structured MREs using physics-augmented neural networks (PANNs) [1,2]. The framework begins with data generation, where a representative volume element (RVE) undergoes macroscopic magneto-mechanical loadings in Finite Element (FE) simulations. The resulting homogenized microscale variables form a macroscale dataset for the training and testing of the PANN macromodel, which satisfies key physical principles [1]. Finally, the trained PANN model is used in a decoupled multiscale scheme as the material model for a macroscale FE simulation to examine the magnetostriction of a spherical sample.

We acknowledge support by the German Research Foundation DFG through Research Unit FOR 5599 on structured magnetic elastomers.

[1] H.T. Roth et al., arXiv:2510.24197, 2025. [2] K.A. Kalina et al., CMAME 421, 2024.

CPP 24.3 Tue 12:00 ZEU/0255

In Silico Self-Assembly of Magnetic Colloidal Polymers with Magnetization Dynamics — •Deniz Mostarac[1], Sofia Kantorovich[2], and Philip J. Camp[1] — [1]School of Chemistry, University of Edingburgh, EH9 3FJ Edinburgh , United Kingdom — [2]Computational and Soft Matter Physics, University of Vienna, Vienna, Austria

Polymer-like mesostructures formed by crosslinked magnetic nanoparticles (MNPs) have created a new class of stimuli-responsive materials magnetic colloidal polymers (MCPs) that show enhanced optical, thermal, mechanical, rheological, and adsorption properties compared to conventional magnetic fluids. The interplay between magnetic interactions and solvophilic/solvophobic forces produces complex, field-tunable self-assembly. In our previous work, we investigated isolated MCPs and showed that solvophobicity drives compact, magnetically frustrated conformations, with structural features determined by crosslink type and MNP properties. These distinctions strongly affect MCP dynamics under shear and external fields. In this contribution we study the self-assembly of solvophobic MCPs while explicitly modeling MNP magnetodynamics with finite anisotropy. Our simulations capture internal magnetization dynamics over long times and at system sizes sufficient for bulk behavior. We show that coupling between Brownian and Néel relaxation, together with nonlinear magnetization, yields distinct structural, magnetic, and dynamical features in MCP suspensions governed by solvophobicity and intrinsic NP magnetism.

CPP 24.4 Tue 12:15 ZEU/0255

Pulling knotted polymer rings and concatenated knotted polymer rings in order to understand the effects of entanglement on the mechanical properties of polymers materials — •Franco Ferrari[1], Neda Abbasi Taklimi[1], Marcin Piatek[1], and Luca Tubiana[2] — [1]CASA* and Institute of Physics, University of Szczecin, Szczecin, Poland — [2]Physics Department, University of Trento, Via Sommarive 14, Trento I-38123, Italy

The topological structure of polymers is expected to produce relevant effects on the mechanical properties of polymer systems. However, to assess the contribution of topology by experiment is difficult, mainly due to technical obstacles in controlling the entanglement during the synthesis process, in particular the formation of knots and concatenations. In this contribution presented are the results of numerical simulations focusing on the mechanical properties of topologically entangled polymer systems. First, the case of single knotted polymers pulled by an external force are discussed. Next, the stress-strain curves of a few concatenated knots with forces applied at different locations are shown. To check the validity of our simulations based on the Wang-Landau algorythm, two different methods are employed and their consistency is verified. The final goal of this research is to understand the mechanical properties of more complex polymer materials characterized by an uniform distribution of knots or concatenated knots of a given topological type.

CPP 24.5 Tue 12:30 ZEU/0255

Prediction of Ultra-Long Time-Scale Dynamics from Picoseconds to Seconds: Integral of First-Passage Times — •Qiyun Tang — School of Physics, Southeast University, Nanjing, China

The dynamics of non-equilibrium nanostructure formation span over 13 orders of magnitude in time, from molecular vibrations at picoseconds to macroscopic processes at seconds or longer. Predicting such ultra-long time-scale dynamics poses significant challenges for conventional molecular simulation methods. We recently proposed a new approach-Integral of first-passage times (IFS)-to predict the evolution of non-equilibrium nanostructures, and the resulting structural distributions align well with experimental observations [1]. Furthermore, we have verified that the dynamics predicted by IFS are consistent with direct simulations in cases of low free energy barriers, while under high free energy barriers, the ultra-long time-scale dynamics predicted by IFS agree with experimental measurements [2]. Utilizing this method, we have also systematically investigated the relationship between polymer adsorption dynamics and surface curvature [3,4]. The IFS method bridges microscopic picosecond-scale dynamics with macroscopic growth kinetics of nanostructures, offering an effective approach for designing and controlling non-equilibrium nanostructures.

[1]Q.Tang, C. Rossner, P. Vana, M. Müller, Biomacromolecules 2020, 21: 5008. [2]Q. Tang, Y. Huang, M. Müller, Phys. Rev. E 2024, 110: 044502. [3]J. Zhang, Q. Tang, Phys. Rev. Mater. 2024, 8: 105602. [4]Y. Huang, C. Tang, Q. Tang,*Nanoscale 2024, 16: 19806.

CPP 25: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics II

Time: Tuesday 11:30–12:45 Location: ZEU/0260

CPP 25.1 Tue 11:30 ZEU/0260

Transiently Delocalised Hybrid Quantum States are the Gateways for Efficient Exciton Dissociation at Organic Donor-Acceptor Interfaces — •Filip Ivanovic[1], Samuele Giannini[2], Wei-Tao Peng[3], and Jochen Blumberger[1] — [1]Department of Physics and Astronomy, University College London, London, United Kingdom — [2]Department of Chemistry and Industrial Chemistry, University of Pisa, Pisa, Italy — [3]Department of Chemistry, Tunghai University, Taichung City, Taiwan

Organic solar cells (OSCs) have long been the subject of intensive research. Following the absorption of sunlight, localised excitations (excitons) are able to dissociate into separated charges at the interface between donor and acceptor components. Whilst this separation has been leveraged to achieve cell efficiencies above 20%, the exact mechanism by which this occurs remains without consensus.

Theoretical research has been centred on simulating such phenomena on experimentally relevant time scales, whilst sufficiently describing the underlying electronic structure. Here, we introduce our in-house non-adiabatic dynamics package, termed X-SH.

We elucidate the mechanism of ultrafast charge separation in an atomistic OSC junction, where separation is mediated by non-local hybridised states comprising both excitons and separated charges, and in-fact accelerated by non-interfacial exciton dissociation. We then demonstrate that tuning the hybridised states' accessibilities through the density of states can be translated into design rules informing the synthesis of yet more efficient OSCs.

CPP 25.2 Tue 11:45 ZEU/0260

Temperature-Dependent Spin-Sensitive Spectroscopy of Triplet-Exciton Dynamics in TADF OLEDs — •Ahmed Mohamed, Andreas Kohrmann, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

Thermally Activated Delayed Fluorescence (TADF) enables efficient harvesting of triplet excitons through reverse intersystem crossing (rISC) in OLEDs. Previous studies have shown that TADF device operation is dominated by triplet excitons, whose densities exceed singlet and charge carrier densities by several orders of magnitude. A major limitation to TADF efficiency is the non-radiative loss of triplet excitons. Here, we analyze the transient photoluminescence (trPL) and transient electroluminescence (trEL) decays of the blue TADF emitter ν-DABNA hosted in TDBA-Si or mCP. Temperature-dependent trPL/trEL kinetics were modeled using a rate-equation framework. Key triplet-exciton parameters, including the lifetime, diffusion coefficient, diffusion length, and activation energies were extracted by considering both 1st and 2nd order triplet-exciton decay pathways. The spin properties of the triplet exciton were additionally identified using photoluminescence-detected magnetic resonance (PLDMR) measurements on the organic layer stack. Together, kinetic and spin analysis of triplet excitons provide a comprehensive picture of non-radiative quenching to guide future improvements of TADF OLEDs

CPP 25.3 Tue 12:00 ZEU/0260

Modeling the ionization potential and electron affinity in organic semiconductors — •Alexey Gudovannyy and Frank Ortmann — Department of Chemistry, TUM School of Natural Sciences, and Atomistic Modeling Center, Munich Data Science Institute, Technical University of Munich, Germany

Ionization potential (IP) and electron affinity (EA) are essential quantities for characterizing and tuning transport properties of organic semiconducting materials. Computational prediction of these properties under realistic conditions of crystalline or polycrystalline forms remains challenging, as it requires a proper description of all interactions within the bulk material environment. In this work, we present an accurate protocol for computing molecular materials' IP and EA values, using computed gas-phase molecular values corrected via an improved multilevel scheme for describing the materials' environment, where an electronic structure is treated explicitly at the microscopic level, while at larger scales, a continuum model is applied. Special significance will be dedicated to the requirement of accurate reference gas-phase calculations, which we carried out within the GW framework and to demonstrating limitations of prevalent Density Functional Theory (DFT) methods, while preserving feasible computational time demands. The main bottleneck of this approach is the need for an experimental or predicted crystal structure. We will also show how to incorporate reliable structure prediction into it, which opens up possibilities for purely in silico materials design.

CPP 25.4 Tue 12:15 ZEU/0260

Morphological Insights into Spray-Coated Organic Semiconductors — •Shuxian Xiong[1,2], Marie Betker[2,3], Simon Schraad[1,2], Yufeng Zhai[2], Benedikt Sochor[2], Sarathlal Koyiloth Vayalil[2,4], Peter Müller-Buschbaum[1], and Stephan V. Roth[2,3] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Department of Fibre and Polymer Technology, KTH, Stockholm, Sweden — [4]Applied Sciences Cluster, University of Petroleum and Energy Studies UPES, Dehradun, Uttarakhand, 248007, India

Ultrasonic spray coating offers improved scalability for large-scale applications, reduced material waste, and enhanced compatibility with various substrates, making it a more cost-effective solution for the mass production of photovoltaic devices. However, how to simply and efficiently build ordered structural networks is still a critical issue. We investigate the morphological transition of organic semiconductors and their effect on device performance using grazing incidence wide-angle X-ray scattering in traditional fullerene systems. By systematically optimizing spray flow rate and substrate temperature, we effectively tailored the film morphology, enhancing molecular crystallization of PTB7-Th and PCBM, resulting in an improvement in device performance of 9% in air, which is one of the highest device efficiencies currently achieved for spray-coated fullerene acceptor-based organic solar cells, and is equivalent to the device efficiencies of spin-coated fullerene acceptor-based organic solar cells.

CPP 25.5 Tue 12:30 ZEU/0260

Enhancing device performance parameters of organic photodiodes by understanding the thickness dependence of the reverse dark current — •Fred Kretschmer[1], Tianyi Zhang[1], Oskar J. Sandberg[2], Mathias Nyman[2], Karl Leo[1], and Johannes Benduhn[1] — [1]Institute of Applied Physics, TU Dresden, Dresden, Germany — [2]Faculty of Science and Engineering, Åbo Akademi University, Turku, Finland

In recent years, organic photodetectors (OPDs) have attracted interest due to their advantageous properties and rapidly advancing performance, making them promising not only as complements to inorganic photodetectors but also for emerging applications in bioimaging, health monitoring, and high-speed optoelectronics. A key figure of merit for comparing PDs is the specific detectivity (D^*), which quantifies the detector's ability to sense weak optical signals. Achieving high D^* relies on maximizing charge carrier extraction while minimizing internal noise. Under reverse bias, OPD performance is particularly influenced by shot noise, which is proportional to the dark current (J_D).

In this work, the variation of J_D with active-layer thickness across multiple energy-gap-tuned bulk-heterojunction systems was examined. Surprisingly, the dark current exhibits a thickness-dependent minimum, contrary to the general assumption that J_D only decreases with thickness. Using sensitive, temperature-dependent current-voltage measurements together with drift-diffusion simulations, the new minimum feature was confirmed, and improvements in the specific detectivity of OPDs were achieved.

CPP 26: French-German Session: 2D Materials, Thin Films and Interfaces II

Time: Tuesday 14:00–15:30 Location: HÜL/S386

Invited Talk CPP 26.1 Tue 14:00 HÜL/S386

Investigating lignin graphitisation depending on botanical source and extraction method — Lucie Dieval[1], Phuthiphong Ouitrakoon[2], Robert Hunter[2], Sébastien Schaefer[3], Louis Hennet[3], Erik Elkaim[4], Julie Ruellou[5], Milo S. P. Shaffer[2], Agnieszka Brandt-Talbot[2], and •Pascale Launois[1] — [1]LPS, CNRS/Université Paris Saclay, France — [2]Imperial College, UK — [3]ICMN, CNRS/University of Orléans, France — [4]Synchrotron SOLEIL, France — [5]ESRF, France

Lignins, plant-derived macromolecules, are promising carbon sources from a sustainable development perspective. Here, we study the transformations of various lignins into turbostratic carbon or graphite, consisting of stacked graphene sheets.

The lignin powders were heated at temperatures between 1000 and 2730°C. Analyses were performed ex-situ using X-ray scattering (XRS) and Raman spectroscopy, which confirmed XRS results. XRS data were analysed combining analyses in reciprocal space and in direct space with Pair Distribution Function. The dimensions of the carbonaceous crystalline domains formed from lignins are determined as a function of temperature, as well as the stacking mode of their graphene sheets. We find that all studied lignins transform into turbostratic carbon, with no evidence for intermediate stackings towards graphite. Different sizes of crystalline domains are evidenced depending on the lignin form. One lignin presents relatively large sizes both for the graphene layers and in the stacking direction at a temperature as low as 1300°C, a most promising finding for future applications.

CPP 26.2 Tue 14:30 HÜL/S386

Atomistic Origin of Photoluminescence Quenching in Colloidal MoS_2 and WS_2 Nanoplatelets — •Surender Kumar[1], Markus Fröhlich[2], Stefan Velja[1], Marco Kögel[2], Onno Strolka[2,3], André Niebur[3], Samuell Ginzburg[4], Muhammad Sufyan Ramzan[1], Jannik C. Meyer[2], Jannika Lauth[2,3], and Caterina Cocchi[1] — [1]Friedrich-Schiller-Universität Jena, Germany — [2]Eberhard Karls University of Tübingen, Germany — [3]Leibniz University of Hannover, Germany — [4]University of Cambridge, UK

Large chemical tunability and strong light-matter interactions make colloidal transition metal dichalcogenide nanostructures particularly suitable for light-emitting applications. However, ultrafast exciton decay and quenched photoluminescence limit their potential. Combining femtosecond transient absorption spectroscopy with first-principles calculations on MoS_2 and WS_2 nanoplatelets, we reveal that the observed sub-picosecond exciton decay originates from edge-located optically bright hole traps [1]. These intrinsic trap states stem from the metal *d*-orbitals and persist even when the sulfur-terminated edges are hydrogen-passivated. Notably, WS_2 nanoplatelets show more localized and optically active edge states than their MoS_2 counterparts, and zigzag edges exhibit a higher trap density than armchair edges. The nanoplatelet size dictates the competition between ultrafast edge-trapping and slower core-exciton recombination, and the states responsible for exciton quenching enhance catalytic activity.

[1] S. Kumar, et al., arXiv:2511.19077 (2025)

CPP 26.3 Tue 14:45 HÜL/S386

Data-driven exploration of thermal and elastic properties in covalent organic framekworks — •Aleksander Szewczyk[1], Leonardo Medrano Sandonas[1], David Bodesheim[1], Bohayra Mortazavi[2], and Gianaurelio Cuniberti[1] — [1]TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Leibniz Universität Hannover, Welfengarten 1A, 30167 Hannover

Covalent organic frameworks (COFs) are a class of advanced materials that can be precisely engineered for diverse applications, including catalysis, flexible electronics, and sensors. However, COFs synthesised experimentally often exhibit a variety of structural defects and grain boundaries, which affect their properties. Because of their large and complex structure, COFs pose a considerable challenge for traditional *ab-initio* methods. Machine learning interatomic potentials (MLIPs) can be used to significantly accelerate property calculations, while retaining near *ab-initio* accuracy. Our team have parametrised an MLIP using the MACE architecture and a dataset of non-equilibrium confirmations of 2D COFs. We assessed the transferability of the MACE model computing atomic forces and phonon dispersions of unseen COFs, and compared these results to ReaxFF and reference data by Density Functional Theory using VASP code. Using the parametrised model, we explore the effect of defects and grain boundaries on thermal and elastic properties of COFs.

CPP 26.4 Tue 15:00 HÜL/S386

PNIPAM Microgel-Stabilized Foam Films: Effect of Crosslinking Content — •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, the 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, characterized by network-like, several 100nm thick regions containing MGs, interspersed with thin MG-depleted zones less than 100nm thick. We show how the cross-linker density of the microgels affect the MG layering within these thick network regions, influencing the film thickness. Another question we answer is how the MG-free areas are stabilized.

CPP 26.5 Tue 15:15 HÜL/S386

Irreversible protein adsorption on mobile surfaces: control and modelling of surface density and in-plane mobility through molecular crowding — Wanchung Chiang[1], Lionel Bureau[1], Ralf Richter[2], Galina Dubacheva[1], and •Delphine Debarre[1] — [1]Grenoble-Alpes University, France — [2]University of Leeds, UK

Adsorption of proteins onto surfaces has been the focus of a wealth of experimental, theoretical and numerical studies but surprisingly little is known on the dynamics of protein adsorption on fluid surfaces.

In this study, we consider irreversible adsorption of streptavidin, a protein with a very strong affinity for its ligand biotin, onto a lipid bilayer incorporating biotin-terminated lipids, a widely-used model to build biomimetic surfaces. We show that after the initial, rapid adsorption phase, a slower, logarithmic continuous adsorption can lead to surface densities much larger than in the absence of surface diffusion. Simultaneously, we quantify the lateral diffusion of the adsorbed proteins, which drops sharply and can be tuned continuously over two orders of magnitude depending on surface density.

We then adapt free-volume theories to two dimensions to rationalize our findings and bridge the gap between in-plane diffusion and adsorption dynamics. Beyond a better understanding of adsorption onto mobile surfaces, our data paves the way towards biomimetic surfaces incorporating mobility control of functional groups.

CPP 27: Focus Session: Water – from Atmosphere to Space III (joint session CPP/DY)

Time: Tuesday 14:00–15:30 Location: ZEU/LICH

Topical Talk CPP 27.1 Tue 14:00 ZEU/LICH

Why water in plants survives negative pressure — Marin Šako[1,2], Emanuel Schneck[3], Roland Netz[4], and •Matej Kanduč[1] — [1]Jožef Stefan Institute, Ljubljana, Slovenia — [2]University of Ljubljana, Faculty of Mathematics and Physics, Ljubljana, Slovenia — [3]Physics Department, Technische Universität Darmstadt, Darmstadt, Germany — [4]Fachbereich Physik, Freie Universität Berlin, Berlin, Germany

It may seem surprising that we can lower the pressure in a liquid to negative values, far below the saturated vapor pressure at which a vapor phase should form. In water, such deeply metastable states are possible only when it is exceptionally pure and free of nucleation sites. It is therefore even more striking that plants transport water at negative pressures down to -100 atm without cavitation, even though xylem sap is anything but pure: it contains dissolved ions, sugars, lipids, and other organic molecules. How is this possible?

In this talk, I will show how molecular simulations and theory can explain this surprising behavior. We find that amphiphilic molecules such as lipids can adsorb onto hydrophobic surface crevices — places that would normally trap nanobubbles. Once coated, these surface defects can no longer stabilize bubbles, which allows water to stay intact even under strong tension. This mechanism offers a molecular-level explanation for how trees transport water to heights of over 100 meters without cavitation. More broadly, it illustrates how soft-matter physics and interfacial molecular organization can control the mechanical stability of liquids under extreme conditions.

CPP 27.2 Tue 14:30 ZEU/LICH

Cholesterol Controlled Photo-Switching Activity of Azobenzene Glycoconjugates in Lipid Membranes — •Prashant Hitaishi[1,2], Svenja C. Hövelmann[1,2], Michael Röhrl[3], Nicolas Hayen[1], Ella Diebell[1], Ali Ashtiani[1], Carlotta Mager[1], Thisbe Lindhorst[3], and Bridget M. Murphy[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, Leibnizstraße 19, Kiel, 24118, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, Hamburg, 22607, Germany — [3]Otto Diels-Institut für Organische Chemie, University of Kiel, Germany

Reversible photo-switchable molecules enable precise optical control of soft interfaces and are attractive for smart surfaces and light-triggered drug delivery. Azobenzene glycoconjugates (Azo) undergo reversible trans-cis isomerization under alternating UV and visible illumination, thereby modulating their conformation and interactions with lipid membranes. Here, Azo is incorporated into DPPC monolayers containing 0, 15, or 30 mol% cholesterol to mimic biologically relevant membrane compositions. Langmuir monolayer isotherm studies combined with time-resolved illumination cycles and X-ray measurements are used to quantify Azo-induced changes in membrane structure and relaxation kinetics. Increasing cholesterol slows Azo photo-switching, indicating a more constrained, rigid nanoenvironment, and shows that membrane composition can be used to tune light responsiveness in lipid interfaces for designing azobenzene-based responsive biomaterials.

CPP 27.3 Tue 14:45 ZEU/LICH

Photoelectron Angular Distributions of Ions Influenced by Surfactants at the Solution-Vapor Interface — •Shirin Gholami[1], Tillmann Buttersack[1], Clemens Richter[2], Rémi Dupuy[3], Daniela Torres-Díaz[1], Christophe Nicolas[4], Uwe Hergenhahn[1], and Hendrik Bluhm[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]SPECS Surface Nano Analysis GmbH, Berlin, Germany — [3]Sorbonne Université, CNRS, Paris, France — [4]Synchrotron SOLEIL, Paris, France

Aqueous liquid-vapor interfaces play key roles in atmospheric and oceanic processes. The ocean-air boundary forms the largest aqueous-vapor interface, covering over 70 % of Earth's surface. In addition to Na^+ and Cl^-, Mg^{2+} and SO_4^{2-} are the most abundant ions in ocean water.

Here, we investigate how Mg^{2+} and SO_4^{2-} ions behave at the aqueous solution-vapor interface in the presence of charged surfactants. Using sub-monolayer coverages of octylamine $-CNH_3^+$ and octanoate $-COO^-$, we examine how these surfactants modify the distance of the ions from the interface. Liquid-jet X-ray photoelectron spectroscopy in combination with photoelectron angular distributions provides Å-scale depth sensitivity, enabling us to quantify ion-surfactant interactions.

Our results show that differently charged surfactants shift the interfacial positioning of Mg^{2+} and SO_4^{2-}, and that specific ion-ion interactions influence their interfacial propensity.These findings reveal how surfactants govern the depth distribution of ions, providing insight into oceanic and atmospheric processes.

CPP 27.4 Tue 15:00 ZEU/LICH

Contact line dynamics on moving fibers measured by X-ray holography — •Louisa E. Kraft[1,2], Jens Lucht[3], Fiona Berner[1,2], Hannes P. Hoeppe[3], Tobias Eklund[1,2], Yizhi Liu[1], Markus Osterhoff[3], Tim Salditt[3], Hans-Jürgen Butt[1], and Katrin Amann-Winkel[1,2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Johannes Gutenberg University, Institute for Physics, Mainz, Germany — [3]Georg-August-University, Institute of X-ray Physics, Göttingen, Germany

The wetting properties of solid surfaces are important for many natural and industrial processes, especially with respect to dynamic wetting. The wetting dynamic of solid surfaces, in particular the quantitative description of the dynamic contact angles, is still under debate. Dynamic contact angle variations connect macroscopically measured quantities with microscopic processes. Most studies rely on optical or confocal microscopy which limits the experimental access to the submicroscopic region where these processes take place. We present data from X-ray holography experiments, imaging the three-phase contact line on moving glass fibers with an improved spatial resolution of about 450 nm combined with a temporal resolution of 10 Hz. We used the GINIX nanofocusing setup at the P10 beamline at PETRA III (DESY, Hamburg). The used glass fibers were pulled out of a liquid bath filled with varying aqueous solutions while changing the lateral velocity. We could clearly observe a decrease of the receding dynamic contact angle with increasing fiber velocity confirming the predictions of dynamic wetting theory.

CPP 27.5 Tue 15:15 ZEU/LICH

Properties of micrometre-sized supercooled water droplets — Claudia Goy[1], •Frédéric Caupin[2], Felix Lehmkühler[1], and Robert E. Grisenti[3,4] — [1]Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — [2]Université Claude Bernard Lyon 1, Villeurbanne, France — [3]GSI, Darmstadt, Germany — [4]J. W. Goethe-Universität, Frankfurt am Main, Germany

Water displays a wide range of anomalous behaviors, many of which become particularly pronounced in the supercooled state, where its properties deviate strongly from those of other liquids. A prevailing hypothesis suggests that, at low temperatures, water may locally adopt two distinct structural motifs. This presentation will discuss results from temperature-dependent experiments that probe the physical and chemical properties of liquid water. The studies employ evaporatively cooled liquid jets in vacuum, investigated with techniques such as Raman spectroscopy and X-ray spectroscopy. These approaches enable a detailed examination of inter- and intramolecular vibrational modes, providing insight into the molecular dynamics of cooling water and optical properties, including the refractive index. Together, these experimental methods offer a comprehensive view of the temperature-dependent behavior of water, shedding light on the complex interactions that drive its anomalies. Through these studies, we aim to elucidate the mechanisms governing water's unique behavior in the supercooled regime and contribute to a deeper understanding of its structural transformations and physical properties.

CPP 28: Active Matter IV (joint session DY/BP/CPP)

Time: Tuesday 14:00–15:30 Location: ZEU/0160

CPP 28.1 Tue 14:00 ZEU/0160

Automated decision-making by chemical echolocation in active droplets — •Aritra K. Mukhopadhyay[1], Ran Niu[2], Linhui Fu[2], Kai Feng[2], Christopher Fujta[1], Qiang Zhao[2], Jinping Qu[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 that enables synthetic microswimmers, including 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, producing echoes that encode structural information about the environment. These echoes trigger automatic responses, such as synthetic chemotaxis, allowing swimmers to avoid dead ends and autonomously find paths through complex mazes. We show the mechanism remains robust across different maze geometries, ensuring reliable navigation without external cues. Our findings illustrate how simple physical principles can endow synthetic systems with advanced navigation functionalities.

CPP 28.2 Tue 14:15 ZEU/0160

Dead or alive?—Probing scale-dependent liveliness in multiscale active matter — •Joscha Mecke[1] and Klaus Kroy[2] — [1]Institute for Advanced Study, Shenzhen University, Shenzhen, China — [2]Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany

If you have ever watched live and dead trouts swimming upstream, side by side, you may have wondered how closer inspection of their mesoscale activity might help to tell them apart. But probing spatially heterogeneous activity in living matter is a major challenge. We demonstrate the emergence of multiple effective ("active") temperatures in nonequilibrium molecular- and Brownian-dynamics simulations of an active polymer. Energy injection at different length scales leads to mode coupling, inter-modal energy transfer, and entropy production. We put forward a generalised Langevin equation for a labelled monomer, which, by application of a harmonic potential, can serve as a spectroscopic device. Upon varying the trap stiffness, we can selectively scan through the emergent effective temperatures and thereby resolve the scale-dependent activity. Our approach thus provides a minimally invasive spectroscopic tool to generate quantitative maps of liveliness, across multiple scales.

CPP 28.3 Tue 14:30 ZEU/0160

Tuning the velocity of thermophoretic microswimmers with thermo-sensitive polymers — Franziska M. Braun, Aritra K. Mukhopadhyay, Samad Mahmoudi, Benno Liebchen, and •Regine von Klitzing — Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstrasse 8, 64289 Darmstadt

Understanding and controlling the motion of self-propelled particles in complex fluids is crucial for applications in targeted drug delivery, microfluidic transport, and the broader field of active matter. Here, we investigate the thermophoretic self-propulsion of partially gold-coated polystyrene Janus particles (Au-PS) in temperature-responsive linear Poly(N-isopropyl acrylamide) (PNIPAM) solutions across various PNIPAM concentrations and temperatures. Particle velocities are examined at three representative temperatures: far below, near but below and above the LCST. In pure water, Au-PS Janus particles propel with the PS hemisphere leading, driven by their intrinsic thermophoretic response. Conversely, the positive Soret coefficient of PNIPAM results in depletion forces that induce motion of the Janus particle towards the hot Au side. The experiments reveal a non-monotonic dependence of particle velocity on temperature, with a maximum near the LCST. Interfacial processes like ion movement in the electric double layer and PNIPAM adsorption at the Au-PS particles are separated from processes that are coupled to the bulk solution. Theoretical calculations are in good agreement with the experimental findings and are essential for the understanding of the complex interplay of microswimmers with thermoresponsive polymers.

CPP 28.4 Tue 14:45 ZEU/0160

Non-reciprocal multifarious self-organization — •Saeed Osat[1] and Ramin Golestanian[2] — [1]Institute for Theoretical Physics IV, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany — [2]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Goettingen, Germany

Biological systems exhibit a unique ability to design diverse structures from a shared set of building blocks, with a plethora of proteins made from a limited set of amino acids as a prime example. Furthermore, these systems often use building blocks efficiently by introducing transformations between different structures. A structure might undergo structural transformations to form a new structure with different functional purposes, without the need to discard the current structure and start anew. To unravel this mystery, one must examine the underlying non-equilibrium processes that make this shape-shifting behavior feasible.

Here, we leverage non-reciprocal interactions between building blocks to provide a foundation for designing dynamic structures. We used a multifarious self-assembly (MSA) model, which is the molecular counterpart of the Hopfield associative memory. By upgrading the MSA model to its non-equilibrium counterpart with non-reciprocal interactions, we introduce the ability to not only self-assemble different structures on demand but also facilitate shifts and transformations that lead to shape-shifting behavior.

Invited Talk CPP 28.5 Tue 15:00 ZEU/0160

Designing topological edge states in bacterial active matter

— Yoshihito Uchida[1], Daiki Nishiguchi[2,1], and •Kazumasa A. Takeuchi[1] — [1]The University of Tokyo, Tokyo, Japan — [2]Institute of Science Tokyo, Tokyo, Japan

Besides its potential relevance to the life sciences, active matter also manifests as a novel, intrinsically non-equilibrium kind of matter, endowed with characteristic transport properties distinguished from conventional matter. A challenge is how to control and design transport in active matter. A potentially useful, emerging concept here is topological transport developed in condensed matter physics, which was extended to active matter successfully, but experimental realizations have thus far relied on the chirality of the active particles, which limits design capabilities.

Here we report a controlled realization of topological edge states in dense bacterial suspension, induced by microfabricated geometry instead of the bacteria's chirality. First we demonstrate that we can rectify bacterial collective motion by a channel with asymmetric shape. Then we construct networks made of asymmetric channels and show that we can control the emergence of topological edge states through the network design. Through modelling and experiments, we discuss what properties of the network and the bacterial flow are crucial to the observed topological phenomenon. We expect our results may pave the way for establishing a control and design principle of topological transport in such active matter systems.

Ref) Y. Uchida, D. Nishiguchi, and K. A. Takeuchi, to appear.

CPP 29: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods III

Time: Tuesday 14:00–15:30 Location: ZEU/0255

CPP 29.1 Tue 14:00 ZEU/0255

Towards Evolved Sensing Applications for Organic Photonic Devices Utilizing Room-Temperature Phosphorescence — •Sebastian Kaiser, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics (IAP), Technische Universität Dresden

Photonic devices function through the absorption and emission of light, making them independent of electricity or other influences. This trait is vital for sustainable advances in imaging, sensing, information storage, and anticounterfeiting. Programmable luminescent tags (PLTs) exemplify this by utilizing the oxygen-sensitivity of organic room-temperature phosphorescence (RTP) for controllable switching of the device's light output under UV illumination. [1, 2]

Optimizing the homogeneity and reproducibility of photonic thin-film devices, paired with use-case-tailored layer compositions, allowed us to develop a new, advanced UV light-sensing application. The thin-film nature of PLTs, especially their flexibility and transparency, combined with a freely scalable sensor area, enables a broader range of use cases than common detectors can achieve. The combination of these unique device characteristics opens the way for new sensing applications for purely photonic devices.

[1] Gmelch et al., Science Advances 2019. aau7310
[2] Tsiko et al., Communications Chemistry 2025, 025-01620-0

CPP 29.2 Tue 14:15 ZEU/0255

Synergistic and unique information reveals multicentre bonding and geometry — •Kyunghoon Han, Miguel Galleogos Gonzalez, and Alexandre Tkatchenko — University of Luxembourg, Luxembourg, Luxembourg

Classical bonding measures and entropy maps are mostly pairwise, obscuring cooperative effects. We introduce a Partial Information Decomposition of bond character built from standard density-functional and coupled-cluster data. Fragment electron- and spin-number distributions along a coordinate define a simple label (covalent, ionic, multicenter), and information about that label is separated into redundant (shared), unique (single-fragment), and synergistic (joint-only) parts. Treating bond character as a geometric response, small perturbations yield a synergy profile that pinpoints where cooperation emerges and how it evolves. The profile rises at the onset of sharing in diatomic hydrogen, is maximal for the central bond of bicyclo[1.1.1]propellane only when the bridgeheads and the three methylene groups are taken together, and peaks at the square geometry of cyclobutadiene before dropping with bond alternation. Benchmarks against density, orbital, energy, and machine-learning descriptors show where PID adds explanatory power and, for ordinary two-center bonds far from dissociation, why it is near-zero with detectable exceptions only when the two atoms are the same.

CPP 29.3 Tue 14:30 ZEU/0255

Utilizing Immediate Phosphorescence in Organic Photonic Devices for Rewritable Information Storage and Oxygen Sensing — •Lucy Winkler, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics (IAP), Technische Universität Dresden

Programmable luminescent tags (PLTs) are photonic devices that offer simple and versatile solutions for reversible information storage and food labeling by using the oxygen-sensitive phosphorescent emission from organic emitters embedded in polymer matrices [1]. Conventional PLTs fabricated by spin-coating under ambient conditions exhibit oxygen-quenched phosphorescence in their initial state, requiring photoactivation to consume oxygen in the active layer and switch on emission. However, these PLTs show inconsistent activation between the initial and subsequent writing processes, significantly limiting their controlled reusability for practical applications [2]. To better understand activation cycles and identify potential improvements, different fabrication workflows in oxygen-free environments were tested. While activation behavior remains similar to conventional devices, these fabrication approaches enable creation of activated PLTs with an initial switched-on state that could serve as simple oxygen detectors, for example, in vacuum packaging integrity monitoring.

[1] Thomas, H. et al. Adv. Mater. 36, 2310674 (2024).
[2] Tsiko, U., et al. Commun Chem 8, 274 (2025).

CPP 29.4 Tue 14:45 ZEU/0255

Solution to the current paradox of anomalous underscreening in electrolytes — •Esther Ohnesorge, Thomas Tilger, Michalis Tsintsaris, Hayden Robertson, and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

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

For aqueous electrolyte solutions, 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. Whilst the surface force apparatus (SFA) provides clear evidence for a re-entrance of repulsion in the highly concentrated regime (termed underscreening) for a wide range of different electrolytes [1], similar observations were not possible with the atomic force microscope (AFM) to date [2]. In this presentation we will examine the reason of these fundamental differences. Specifically, in an attempt to explore experimental screening lengths across a wide suite of electrolyte concentrations, we demonstrate the experimental parameters dominating the occurrence of anomalous underscreening and a comprehensive understanding of this long-debated phenomenon. [1] DOI: 10.1103/PhysRevLett.119.026002 [2] DOI: 10.1016/j.jcis.2022.05.004

CPP 29.5 Tue 15:00 ZEU/0255

Thermal properties of a knotted diblock copolymer ring — •Neda Abbasi Taklimi[1], Franco Ferrari[1], Marcin Radoslaw Piatek[1], and Luca Tubiana[2] — [1]Institute of Physics, University of Szczecin, Wielkopolska15, 70-451 Szczecin, Poland — [2]INFN-TIFPA, Trento Institute for Fundamental Physics and Applications, Via Sommarive 14, I-38123 Trento, Italy

The phase transitions and geometrical properties of diblock copolymers have been studied extensively; however, few studies have addressed knotted structures under varying monomer distributions and solvent quality. Here, we present a computational study of how topological constraints and block lengths affect the behavior of a single diblock copolymer ring. We used the Wang-Landau Monte Carlo algorithm and a coarse-grained model on a simple cubic lattice with an implicit solvent to explore thermal and structural properties. In the AB model, A-type monomers are self-repulsive, B-type monomers are self-attractive, and AB interactions are neutral; the solvent is good for A-type and poor for B-type monomers at low temperatures.

We computed key properties, including heat capacity, radius of gyration of individual blocks and the whole ring, number of contacts (AA, BB, AB), and knot length. Our results reveal several phase transitions for specific monomer distributions and topologies. Subtle changes in monomer distribution lead to transitions between knotlocalization and delocalization at low temperatures, driven by the competition between entropic and energetic contributions to the free energy.

CPP 29.6 Tue 15:15 ZEU/0255

A Systematic Multiscale Study of Bio-Based Polymers for Novel Food Packaging Systems — •Andoni Ugartemendia, Alessandro Mossa, and Giorgia Brancolini — Institute of Nanoscience, CNR-NANO S3, via G. Campi 213/A, 41125 Modena, Italy

Recently, monolayer materials of bio-based polymers have gained increased attention to develop more sustainable packaging systems.[1] In this regard, rational in silico design has become essential to predict novel polymers and reduce experimental workload. However, the computational modeling of these materials poses a great challenge since their dynamics span over different time scales.[2] To bypass this issue, in this work we propose a modular multiscale computational protocol to study linear polymers from ab initio to coarse grained (CG) dynamics. In the first part, we derive a full atomistic force field (FA-FF) from DFT data and carry out FA-MD simulations for its validation. In the second step, all structural properties are passed to a database to parametrize a CG-FF with the iterative Boltzmann inversion (IBI).[3] Lastly, large scale CG-MD simulations are run for a final validation of the CG-FF. This methodology is applied first to PET, a polymer widely used in the packaging industry, as well as to emerging bio-based polymers such as PEF and PLLA.

[1] V. Guillard, et al., Front. Nutr., 2018, 5, 121. [2] R. B. Bird, R. C. Armstrong, O. Hassager, Dynamics of Polymeric Liquids. Volume 1: Fluid Mechanics, 2nd ed. (Wiley-Interscience, United States, 1987). [3] A.P. Lyubartsev, et al., J. Chem. Theory Comput. 2013, 9, 1512.

CPP 30: Complex Fluids, Colloids, Micelles and Vesicles I

Time: Tuesday 14:00–15:30 Location: ZEU/0260

Invited Talk CPP 30.1 Tue 14:00 ZEU/0260

Solvent effects on amphiphile self-assembly in Deep Eutectic Solvents — •Karen Edler — Centre for Analysis and Synthesis, Chemistry Department, Lund University, Sweden

Deep eutectic solvents (DES) are mixtures of hydrogen bond donors and acceptors that form strongly hydrogen-bonded room temperature liquids. These mixtures are straightforward to prepare, using cheap, bioderived components, with lower volatility than most organic solvents, so are potential new green solvents for applications from drug delivery to battery electrolytes. We are interested in micelle templating of inorganic nanomaterials and formulations for delivery of actives, using these versatile solvents.

Changing the H-bonding components and their ratios alters the physicochemical properties of DES, leading to changes in solubility of other species in these solvents. This also alters the self-organisation of surfactants in these mixtures. We have investigated how specific DES components and their molar ratios impact upon solubility and structuring in surfactant solutions, using small angle X-ray and neutron scattering and rheology. Factors such as polarity, the presence of water, and the intermolecular interactions, both between solvent components and with the surfactant headgroups, play a role in the size and morphology of the micelles formed. We aim to develop design rules for novel complex solutions with applications in templating, rheology control and encapsulation using these interesting new solvent systems.

CPP 30.2 Tue 14:30 ZEU/0260

Brick by Brick - Magnetic Particle Transport — •Margaret Rosenberg[1], Jonas Bugase[2], Christian Janzen[2], Rico Huhnstock[2], Arno Ehresmann[2], and Hartmut Löwen[1] — [1]Heinrich-Heine University Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf — [2]Institute of Physics , University of Kassel, 34132 Kassel

Facilitated by advances in particle synthesis, anisotropic and anisometric magnetic micro- and nanoparticles have been intensely studied in recent years, as the particles' lack of symmetry can give rise to unique, tailor-able interactions. However, the modeling of off-equilibrium processes in non-trivial magnetic landscapes is still relatively under-explored. This contribution will seek to understand the ratchet-like transport process of a magnetically coated polymer block ("brick") across a stripe-patterned magnetic surface via a sequence of time-dependent external magnetic fields, from a simulation perspective. In particular, we explore the rotational behavior unlocked by the anisotropic particle shape, and discuss the connection to ongoing experiments.

CPP 30.3 Tue 14:45 ZEU/0260

Role of acids in stabilizing Reverse Micelles: the case of Dodecyl Sulfate — •Qixuan Li and Marialore Sulpizi — Faculty of Physics and Astronomy, Ruhr-University Bochum

The anionic surfactant Sodium dodecyl sulfate (SDS) can form reverse micelles (RMs) in two non-miscible components above the critical micelle concentration [1]. Although the RMs in salt or alkali solution has been investigated in previous studies [2,3], less is known on the working mechanism of acids in SDS RMs. Here, we employ all-atom (AA) and coarse-grained (CG) molecular dynamics to investigate the effects of chloroauric acid (HAuCl4), fluoroboric acid (HBF4) and phosphoric acid (H3PO4) solutions on the stability of the RMs through spontaneous self-assembly in toluene. We find that investigated acids can stabilize micellar structure, particularly H3PO4 due to the stable hydrogen-bonds it forms with the SDS headgroups. In addition, HAuCl4 can significantly influence micelle shape because of its strong polarizability at the water-toluene interface, while HBF4 causes the highest interfacial tension as a result of its significant hydrophilicity. Moreover, scission free energy calculations from CG simulations [4,5] reveal important differences, which along with the viscosity can explain how different acids affect the size of RMs. Our findings can help to rationalize the impact of different acids on the RMs stability and morphology and, in turn, on the metallic nanoparticles synthesis where the RMs are used as nanoreactors.

CPP 30.4 Tue 15:00 ZEU/0260

Microsecond-Resolved Tracking of Ultrasound-Responsive Colloids: From Rigid Silica Probes to Acousto-Responsive Microgels — Parsa Kassaiyan, Regine von Klitzing, and •Amin Rahimzadeh — Technische Universität Darmstadt, Hochschulstrasse 8, 64289 Darmstadt, Germany

Dynamic Light Scattering (DLS) is a powerful tool for characterizing dispersed particles, providing access to their size, size distribution, and dynamical behavior. Here, we integrate high-frequency ultrasound excitation into a conventional DLS setup to resolve the microsecond-scale motion of colloidal particles subjected to intense acoustic fields. This enables simultaneous extraction of particle size and ultrasound-induced oscillation parameters such as vibration frequency, amplitude, and acoustic response, through analysis of the scattered-light intensity correlation function. Compact silica particles serve as robust reference probes: their size remains unaffected by ultrasound, allowing us to map local acoustic energy dissipation by tracking their oscillatory motion at varying distances from the ultrasound source. Building on this reference system, we investigate acousto-responsive PNIPAM microgels. We find that microgels undergo a pronounced ultrasound-induced volume phase transition, shrinking due to rapid dehydration driven by absorption of high-frequency acoustic energy. Our approach thus provides both microsecond-resolved characterization of particle dynamics and a direct pathway to understanding, and exploiting, the acousto-responsiveness of microgels.

CPP 30.5 Tue 15:15 ZEU/0260

Influence of End Groups on the Aggregation of Polymers: A Neutron Scattering Study — •Jonathan Linus Samuel Garthe[1,2], Sylvain Prévost[3], and Matthias Karg[1] — [1]Physical Chemistry of Functional Polymers, Martin Luther University Halle-Wittenberg, Halle (Saale), Germany — [2]Physical Chemistry: Colloids and Nanooptics, Heinrich Heine University Düsseldorf, Düsseldorf, Germany — [3]Large Scale Structures, Institut Laue-Langevin, Grenoble, France

The solution structure of polymers depends strongly on polymer concentration, solvent quality, and molecular weight. Additionally the nature of chemically different terminal groups influences the phase behavior of polymers with strong differences depending on the average chain length. We investigated the solution behavior and the occurrence of micelle-like structures for (semi)-dilute solutions. We synthesized PNIPAM homopolymers that are hydrophobically terminated. Via aminolysis we also cleaved the hydrophobic end groups allowing for direct comparison of the same homopolymers with and without hydrophobic end group. Small-angle neutron scattering was used to study the structure of the polymers in solution. Our studies demonstrated that a subdominant micelle formation occurs for samples with molecular weights below 100 kDa. The aggregation number of these micelles scales inverse with the molecular weight. At low concentrations, these micelles exist as individual structures. Upon increasing the concentration micelles aggregate, leading to a distinct structure factor contribution in the scattering profile.

CPP 31: Responsive and Adaptive Systems

Time: Wednesday 9:30–11:30 Location: ZEU/0255

Invited Talk CPP 31.1 Wed 9:30 ZEU/0255
Hydrogels with a Pinch of Embodied Intelligence — •Andreas Walther — Department Chemie, JGU Mainz

Smart is good, but intelligent is better. The next frontier in soft matter research is to design life-like materials with embodied intelligence, featuring the integrated sensor-processor-actuator paradigm. Our work explores how hydrogels and soft robotic systems can be endowed with autonomous operation and decision-making capacity by embedding chemical reaction networks, enzymatic feedback loops, and mechanical gating principles. Such metagels and metamaterials are capable of self-strengthening behavior, strain-gated responses, and non-reciprocal motion, moving far beyond the limits of traditional responsive materials. By intertwining chemical, mechanical, and structural information, these systems provide a blueprint for programmable, adaptive matter that approaches the complexity and functionality of biological tissues.

CPP 31.2 Wed 10:00 ZEU/0255
Secondary crosslinking of thermoresponsive microgels for smart microgel-based membranes — •Jonas Runge[1,2], Stefanie Uredat[1,2], Aditi Gujare[1,2], Domenico Truzzolillo[2], Julian Oberdisse[2], and Thomas Hellweg[1] — [1]Physical and Biophysical Chemistry, Bielefeld University, Germany — [2]Laboratoire Charles Coulomb, Université Montpellier, France

Responsive microgels are crosslinked polymer networks of colloidal size, which undergo a so-called volume phase transition induced by a certain stimulus like e.g. temperature or pH. Temperature sensitive microgels undergo a strong decrease in size at the volume phase transition temperature (VPTT). Smart membranes are based on responsive polymers and allow to open pores triggered by an external stimulus [1]. Our project on smart microgel-based membranes (SmartBRANE) aims to incorporate an UV-crosslinker and form membranes by activating the UV-crosslinker [2]. The working temperature of low-temperature fuel cells is in the range of 80-100 °C. Since the VPTT of common acrylamides is close to the physiological temperature, we synthesized a hydrophilic acrylamide monomer (NIPMAMol) with an extrapolated VPTT of 85°C. In this work, we copolymerize NIPMAMol with NIPAM and the UV-crosslinker HMABP to increase the VPTT of the then formed membrane. The thermoresponsive properties of the microgels are characterized with PCS. The distribution of the UV-crosslinker within the microgels particles and the formed membrane is investigated with contrast-matching SANS experiments. [1]Runge,Gujare,Uredat, PCCP, 2024, 26, 2732.[2]Dirksen, RSC Advances, 2021, 11(36), 22014.

CPP 31.3 Wed 10:15 ZEU/0255
Photoresponsive Control of Fullerene Diffusion in Azo-BT Nanotraps — Dmitry A. Ryndyk[1,2] and •Olga Guskova[1] — [1]IPF Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany

We present a light-switchable azobenzene-bithiophene (Azo-BT) self-assembled monolayer (SAM) on Au(111) that operates as a reversible nanotrap for C60. Using density-functional theory and QM molecular dynamics, we quantify C60 adsorption on planar layers and diffusion on the SAM and within a fixed 12 A slit-like pore. Direct adsorption on the cis layer is about twice as favorable as on the trans layer due to stronger dispersion interactions with exposed thiophene rings, whereas the densely packed trans layer presents mainly hydrogen contacts and weaker binding. In the slit geometry, the trans (and mixed) layers provide an open pore that captures C60, while photoisomerization to cis closes the slit and prevents release. Diffusion analysis shows that specific interaction sites along the slit walls and the effective degree of confinement - arising from local potential variations within the fixed 12 A slit - govern diffusion pathways and escape barriers. External electric fields or charging of the Au/Azo-BT/C60 complex enable active expulsion, offering design principles for light- and field-responsive nanocarbon trapping interfaces. The financial support from DFG (grant number 509039598) is highly appreciated.

CPP 31.4 Wed 10:30 ZEU/0255
Reversible Photoswitching of Arylazopyrazole-functionalized Polyacrylamide Thin Films under Water Vapor — •David P. Kosbahn[1], Morgan P. Le Dû[1], Simon A. Wegener[1], Feifei Zheng[2], Robert Cubitt[3], René Steinbrecher[4], André Laschewsky[4,5], Christine M. Papadakis[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]Institut für Chemie, Universität Potsdam, Potsdam-Golm, Germany — [5]Fraunhofer Institut für Angewandte Polymerforschung, Potsdam-Golm, Germany

This study investigates the swelling behavior of p(AAPEAm-co-DMAm) films in both isomeric states of the novel photoswitchable molecule arylazopyrazole (AAP). The impact of reversible switching using two different wavelengths on swelling of the polymer in water vapor is examined, with the aim of controlling water uptake, expansion, and nanoscale morphology. This material shows potential for applications in reversible light sensors, photo-actuators, and drug delivery systems. We use time-resolved FTIR spectroscopy to monitor group vibrations during switching, gaining insights into molecular interactions throughout the isomerization processes. 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 arylazopyrazole moieties on the polymer's microscopic properties.

CPP 31.5 Wed 10:45 ZEU/0255
Modeling the Viscoplastic Deformation of Azopolymers Under the Influence of Structured Light — •Nikolai Liubimtsev and Marina Saphiannikova — Leibniz Institute of Polymer Research Dresden, Germany

A distinctive feature of side-chain azopolymers is their ability to convert structured light into a well-defined stress field [1]. This field results from the alignment and elongation of polymer backbones along the light-polarization direction, which acts as a nematic director. Linearly or elliptically polarized irradiation induces uniaxial or biaxial chain orientation, and the stress tensor is proportional to the rate of change of the second-order orientation tensor, predicted from the spatial distribution of light intensity and polarization [1]. Using viscoplastic photoalignment modeling, we achieve excellent agreement with experimentally observed reshaping of azopolymer microstructures. Three-dimensional light fields - such as tightly focused Gaussian beams or q-plate patterns - produce directional photodeformations. These fields are incorporated into ANSYS either analytically or by directly mapping intensity, polarization, and ellipticity at each material point, the latter being especially useful for arbitrary SLM-generated patterns. Financial support from DFG grant GR 3725/10-1 is gratefully acknowledged.

References: [1] I. K. Januariyasa, F. Reda, N. Liubimtsev, et al., Stress-driven photo-reconfiguration of surface microstructures with vectorial light fields, arXiv:2506.06857 (2025), accepted for publication in Light: Science and Applications.

CPP 31.6 Wed 11:00 ZEU/0255

Impact of surface chemistry on the adsorption and dynamics of stimuli-responsive polymers — Baptiste Chabaud[1], Wanchung Chiang[1], Lionel Bureau[1], Ralf Richter[2], Rachel Auzély[1], Delphine Debarre[1], and •Galina Dubacheva[1] — [1]Université Grenoble Alpes, Grenoble, France — [2]University of Leeds, Leeds, UK

Stimuli-responsive polymers at interfaces underpin smart coatings, sensors and bioinspired materials, yet how surface chemistry controls their binding and dynamics remains poorly understood. We probe the interfacial behavior of redox- and thermosensitive polymers on well-defined model surfaces using QCM-D, SPR, ellipsometry, electrochemistry and fluorescence microscopy. For redox-active host/guest systems, we show that grafting strategy, linker flexibility and host/guest density govern the stability, specificity and reversibility of polymer assemblies. Kinetic analysis further reveals that small changes in surface chemistry, such as linker design or dilution with inert molecules, strongly tune multivalent superselectivity, enabling sharp discrimination of receptor densities. Using supported lipid bilayers as fluid interfaces, we correlate lateral mobility with contraction, dehydration and 2D aggregation of thermoresponsive polymer brushes. Overall, we identify interfacial density, mobility and flexibility as key parameters for controlling stimuli-responsive polymer assemblies and outline design rules for supramolecular and bio-inspired systems with high specificity and precision.

CPP 31.7 Wed 11:15 ZEU/0255

Modeling of magnetic hysteresis in magneto-active elastomers — •Pawan Patel[1,2], Dirk Romeis[1], and Marina Saphiannikova[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V, Hohe Straße 6, 01069, Dresden, Germany — [2]Faculty of Mechanical Science and Engineering, Dresden University of Technology, 01062, Dresden, Germany

Magneto-active elastomers (MAEs) are soft polymer composites containing magnetizable microparticles. MAEs exhibit field-dependent mechanical and magnetic properties. When subjected to an external magnetic field, MAEs display magneto-mechanical coupling effects such as tunable stiffness and reversible shape changes. This study presents a multiscale theoretical model to describe the magnetic hysteresis behavior of MAEs, focusing on the role of microstructure evolution during magnetization and demagnetization of microparticles. The total energy of the system is formulated as the sum of magnetic and micromechanical contributions, while macroscopic deformation of the cylindrical sample is constrained. The model incorporates both pure dipole–dipole interactions and near field effect to account for multipole higher-order particle interactions. The results reveal that magnetic hysteresis in soft magnetic MAEs arises primarily from microstructural rearrangements, where the spatial configuration of particles differs between increasing and decreasing magnetic fields. Simulations demonstrate that parameters such as particle volume fraction, sample geometry, and micromechanical stiffness significantly influence the hysteresis loop width.

CPP 32: Focus Session: Water – from Atmosphere to Space IV (joint session CPP/DY)

Time: Wednesday 9:30–10:45 Location: ZEU/0260

Topical Talk CPP 32.1 Wed 9:30 ZEU/0260

Synchrotron X-Ray Studies on Structural Transitions in Water and Alcohol containing Ice Analogues — •Christina M. Tonauer — Institute of Physical Chemistry, University of Innsbruck, Austria — Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

To this date, 21 different crystalline and at least 3 distinct amorphous forms of water ice have been discovered. In addition to the structural versatility of pure water ice phases, water forms solid guest-host systems, so-called 'clathrate hydrates' where water builds cage-like structures around guest molecules of various sizes (e.g., Ar, CO2, methane, ethanol).

Ices in space are exposed to various forms of (external) stress, e.g., impacts, cosmic rays, UV/Vis radiation as well as endogenous thermal fluctuations, thereby undergoing structural changes. By studying such structural transitions in ice analogues upon heating (and/or radiation), conclusions can be drawn about the conditions at various extraterrestrial environments.

Therefore, we here present temperature-resolved wide- and small-angle synchrotron X-ray scattering data of vapor-deposited water-ethanol mixtures of various concentrations, collected at PETRA 3/DESY. While the SAXS data allows for monitoring of changes of the morphology of the microporous sample, the WAXS data reveals the formation sequence of two different hydrates, offering new insights into the crystallisation of astrophysical ices.

CPP 32.2 Wed 10:00 ZEU/0260

Water in exoplanetary atmospheres: from molecular spectra to Water Worlds — •Sergey Yurchenko — Department of Physics and Astronomy, University College London, Gower Street, WC1E 6BT London, United Kingdom

Water vapour is one of the key tracers of atmospheric physics and chemistry on exoplanets, from hot Jupiters to temperate sub-Neptunes and so-called Water Worlds. In this contribution I will give an overview of the role of H_2O across this diversity of atmospheres, focusing on how we infer its presence from transmission and emission spectra. I will review both low-resolution transit spectroscopy and high-resolution cross-correlation techniques, and show how they are applied to data from space- and ground-based facilities, including JWST, Hubble and VLT, as well as future observations with the ELT and ESA's Ariel mission. Special emphasis will be placed on the way clouds and hazes imprint themselves on the observed spectra.

I will summarise the current observational status of water detections and non-detections – including recent and sometimes controversial claims for habitable-zone planets. A central theme of the talk will be the importance of accurate laboratory and theoretical data for water and related species. I will highlight how comprehensive molecular line lists and cross sections from the ExoMol and HITRAN databases, together with other laboratory measurements, underpin the modelling and retrieval of exoplanet spectra over a wide range of temperatures, pressures and compositions, thereby linking detailed molecular physics to the emerging picture of water in exoplanetary atmospheres.

CPP 32.3 Wed 10:15 ZEU/0260

Structures of Ices by Quantum Crystallography and PDF — Krzysztof Wozniak[1], •W. Sławiński[1], G. Łach[2], R. Gajda[1], M. Chodkiewicz[1], P. Rejnhardt[1], M. Arhangelskis[1], Ch. Ridley[3,4], and C. L. Bull[3,5] — [1]Deptm. of Chem., Univ. of Warsaw,Poland — [2]Deptm. of Phys., Univ. of Warsaw, Poland — [3]ISIS Neutron and Muon Source, STFC, RAL, Harwell Campus, UK. — [4]Spallation Neutron Source, Oak Ridge Nat. Lab., Oak Ridge, Tennessee 37830, USA — [5]Univ. of Edinburgh, UK.

Ice is the solid form of water (H*O). The most familiar form of ice is the hexagonally structured ice Ih. However, water can crystallize into at least 21 distinct phases, unique in structure, depending on T and P and route of formation. In this contribution, will present details of structures of ices (VI[3], VII[1,2], Ih [4]) obtained with quantum-crystallographic Hirshfeld Atom Refinement against single crystal X-ray and electron diffraction data. We will also present the first quantitative characterisation of disorder in D2O ice VII and VI obtained through a combination of Pair Distribution Function (PDF) analysis, Reverse Monte Carlo (RMC) modelling, and high-pressure neutron scattering. Our results provide a detailed decomposition of both the average and local atomic structures of Ice VII, revealing a previously unquantified level of structural disorder. References [1] R. Gajda et al., IUCRJ, 12(3) (2025) 288-294; [2] W. A. Sławiński et al., Hidden complexity in D2O Ice VII, Acta Mat., (2025) submitted; [3] M. L. Chodkiewicz et al., IUCRJ, 9 (2022) 573-579; [4] M. L. Chodkiewicz et al., IUCRJ, 11(5) (2024) 730-736.

CPP 32.4 Wed 10:30 ZEU/0260

Water dynamics in conductive PEDOT:PSS/cellulose nanocomposite films in dependence of relative humidity and temperature — •Lucas Kreuzer[1], Marie Betker[2], Marcell Wolf[1], Jacques Ollivier[3], Daniel Söderberg[4], and Stephan V. Roth[2,4] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), TUM, Garching, Germany — [2]Deutsches Elektronen Synchrotron, Hamburg, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]Department of Engineering Mechanics, Royal Institute of Technology KTH, Stockholm, Sweden

PEDOT:PSS is a conductive and water-soluble polymer blend widely used in organic electronics. However, pure PEDOT:PSS films absorb significant amounts of water, 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, a minor amount of water is still absorbed, leading to a change in film morphology: high humidity 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. Moreover, at higher temperatures, different diffusive behavior was found for bulk and hydration water.

CPP 33: Complex Fluids, Colloids, Micelles and Vesicles II

Time: Wednesday 10:00–11:15 Location: ZEU/LICH

Invited Talk CPP 33.1 Wed 10:00 ZEU/LICH

Shape-induced superstructure formation in concentrated ferrofluids — •Sabrina Disch — University of Duisburg-Essen, Essen, Germany

The response of magnetic nanoparticles to applied static and dynamic magnetic fields is the subject of intense research in view of its fundamental technological importance [1]. The field-assisted self-organization of shape-anisotropic nanoparticles in dispersions is particularly desired for liquid crystalline or optically anisotropic materials and as a prerequisite for self-organization into long range ordered arrangements [2]. A strong structure-directing influence of the particle shape on the symmetry of mesocrystalline arrangements has been established for nanocubes with a varying degree of cubicity [3].

In this contribution, we give a detailed account on the impact of nanoparticle shape and size on the interparticle correlations in colloidal dispersions of maghemite nanoparticles. Despite the similar particle size, magnetic moment, and volume concentration (>5 vol-%), we observe a significantly distinct aggregation behavior of nanospheres and nanocubes using small-angle neutron scattering [4]. The field-dependent arrangement of cuboidal nanoparticles into mesocrystalline assemblies and their geometric orientation will be discussed as observed by field-dependent small-angle scattering experiments.

[1] Q. A. Pankhurst et al., J. Phys. D: Appl. Phys. 36, R167 (2003).
[2] S. Disch, E. Wetterskog et al., Nano Letters 11, 1651 (2011).
[3] E. Wetterskog, S. Disch et al., Nanoscale 8, 15571 (2016).
[4] P. Bender, S. Disch et al., J. Appl. Cryst. 55, 1613 (2022).

CPP 33.2 Wed 10:30 ZEU/LICH

Modeling artificial cells to control the local chemical environment — •Nils Göth and Joachim Dzubiella — Applied Theoretical Physics—Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany

Living cells change and respond to their environment. Synthesized artificial cells (hollow microgels) show in experiments pH-responsive behavior by a pH-dependent membrane permeability and change their pH-environment by a chemical reaction [1]. Here, we report a simple model for such artificial cells based on the feedback mechanism between permeability and pH. We introduce the model on the basis of recent experiments [1] and study the effects of experimentally tunable parameters. The model captures not only the effects observed in the experiments, but further predicts the behavior of mixtures of two different kinds of artificial cells. Thus, we provide guidance for future experiments in the field of collective behavior of artificial cells.

[1] Krehan et al., Chem 11, 102409 (2024).

CPP 33.3 Wed 10:45 ZEU/LICH

Evaporation-driven assembly of colloidal monolayers and multilayers — •Qingguang Xie[1] and Jens Harting[1,2] — [1]Helmholtz-Institut Erlangen-Nürnberg for Renewable Energy (IET-2), Forschungszentrum Jülich, Erlangen, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Drying of colloidal suspension films is a common approach to synthesize colloidal monolayers and multilayers for applications such as photovoltaics and catalysis. The fundamental understanding of the complex processes involved in film drying is essential for controlling and optimizing the deposition structure. We numerically investigate the drying dynamics of both thin and thick colloidal suspension films. For thin films, we focus on the influence of substrate and particle wettability on assembled monolayers. High substrate wettability promotes hexagonally packed monolayers, while low wettability leads to droplet formation and particle clustering. Furthermore, we reveal that higher particle wettability can mitigate the impact of substrate wettability and facilitate the formation of highly ordered monolayers. We propose theoretical models predicting the surface coverage fraction dependent on particle volume fraction, initial film thickness, particle radius, as well as substrate and particle wettability, and validate these models with simulations. In a further step, we investigate the drying of thick films with different particle-particle interactions. Weak interactions led to densely packed structures, while strong interactions led to more porous structures due to aggregation.

CPP 33.4 Wed 11:00 ZEU/LICH

Microscopic liquid marbles for force sensing using AFM — •Tomas P. Corrales[1], Constanza Rodriguez[1], Catalina Navarrete[1], Diego Cortés[2], Michael Kappl[2], and Syuji Fujii[3] — [1]Universidad Tecnica Federico Santa Maria — [2]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [3]Osaka Institute of Technology, Osaka, Japan

An AFM cantilever is an exceptional tool for measuring friction and adhesion forces at the nanoscale. We have recently shown the possibility of fixing microscopic liquid droplets on the end of a tipless AFM cantilever, which was used to measure friction forces of a Teflon surface (D. Cortes et al., Physical Review Letters 135, 048203, 2025). In this new work, we have set out to extend this approach by fixing microscopic liquid marbles at the end of an AFM cantilever. Liquid marbles are prepared from hydrophobic nanoparticles of CaCO3. We first spray a mixture of water glycerol over a powder of these CaCO3 nanoparticles, which creates a collection of microscopic liquid marbles. Afterwards, we attach these droplets to a hydrophobic tipless AFM cantilever with a hydrophilic sticky point. With this system we explore liquid marble friction, adhesion and stability.

CPP 34: Focus Session: Water – from Atmosphere to Space V (joint session CPP/DY)

Time: Wednesday 11:00–12:00 Location: ZEU/0260

CPP 34.1 Wed 11:00 ZEU/0260

Scalable Machine Learning Model for Energy Decomposition Analysis in Aqueous Systems — •Thomas Kühne — CASUS/HZDR, Görlitz, Germany

Energy decomposition analysis (EDA) based on absolutely localized molecular orbitals provides detailed insights into intermolecular bonding by decomposing the total molecular binding energy into physically meaningful components. Here, we develop a neural network EDA model capable of predicting the electron delocalization energy component of water molecules, which captures the stabilization arising from charge transfer between occupied absolutely localized molecular orbitals of one molecule and the virtual orbitals of another. Exploiting the locality assumption of the electronic structure, our model enables accurate prediction of electron delocalization energies for molecular systems far beyond the size accessible to conventional density functional theory calculations, while maintaining its accuracy. We demonstrate the applicability of our approach by modeling hydration effects in large molecular complexes, specifically in metal-organic frameworks.

CPP 34.2 Wed 11:15 ZEU/0260

Advances in absolute-scale electronic structure measurements of liquid water and aqueous solutions — •Florian Trinter — Fritz-Haber-Institut, Berlin, Germany

Recent advances in liquid-jet photoelectron spectroscopy (LJ-PES) have enabled the precise determination of absolute electronic energetics of liquid water and aqueous solutions, both in the bulk and at interfaces. By implementing refined vacuum and Fermi-level referencing procedures, rooted in condensed-matter concepts, vertical ionization energies (VIEs) and solution work functions can now be measured with high accuracy. We show that binding energy determinations near the ionization threshold are strongly influenced by quasi elastic electron scattering and indirect ionization processes. Vibrational excitation and autoionization via super-excited states lead to spectral distortions at electron kinetic energies below ~14 eV, necessitating careful data interpretation to extract intrinsic properties. Applying these methods to neat water and aqueous solutions of sodium iodide (NaI) and tetrabutylammonium iodide (TBAI), we reveal solute-specific effects: NaI primarily alters water's bulk structure, increasing the $1b_1$ binding energy with concentration, while TBAI affects surface potentials through interfacial dipole formation, leading to an apparent binding energy decrease. Additionally, we determine the work function of neat water as 4.73 ± 0.09 eV and quantify its reduction in TBAI solutions. These findings establish a framework for quantitative studies of molecular interactions and electronic-structure modifications in aqueous systems, with implications for electrochemical and interfacial science.

CPP 34.3 Wed 11:30 ZEU/0260

Liquid-vapor critical behavior of the TIP4P/2005 water model: Effects of NaCl solutes and hydrophobic confinement — •Mayank Sharma and Peter Virnau — Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

The liquid-vapor critical behavior of water is strongly influenced by both ionic solutes and confinement. Molecular dynamics simulations of aqueous NaCl solutions using the TIP4P/2005 water model and the Madrid-2019 ion parameters reveal a systematic increase in the liquid-vapor critical temperature and pressure with salt concentration, consistent with experimental trends. In contrast, confinement between parallel hydrophobic plates leads to a depression of the critical point. The critical temperature was determined using the Binder cumulant crossing in the NVT ensemble, based on a recently developed method originally applied to an active Brownian particle system [1]. The reliability of this approach was verified through complementary NPT simulations using histogram reweighting. We further demonstrate the pronounced sensitivity of the estimated critical point to the van der Waals cutoff distance, underscoring the importance of properly accounting for long-range interactions. The present results capture qualitative shifts in the critical point of water arising from ionic interactions and confinement, and the Binder-cumulant framework used here is readily extendable to other critical phenomena, including the putative liquid-liquid critical point of water.

[1] J.T Siebert et al., Phys. Rev. E 98, 030601 (2018).

CPP 34.4 Wed 11:45 ZEU/0260

Cooperative molecular dynamics and nuclear quantum effects in bulk water — •Margarita Russina — Helmholtz-Zentrum Berlin for Materials and Energy, Berlin, Germany

The cooperative dynamics in water remain difficult to access due to the lack of long-range order and the short lifetimes of molecular correlations. Neutron scattering is well suited to probe such phenomena on the nanoscale but has been hindered by the weak coherent signal of H2O. Using a novel neutron polarization-analysis approach, we directly measure the coherent scattering in H2O and D2O with high accuracy [1]. Beyond self-diffusion and molecular rotation, we identify a picosecond cooperative process in liquid water, likely associated with rearrangements of several neighboring molecules and the reorganization of hydrogen bonds. This process may act as a precursor to large-scale molecular transport. In the intermediate wave-vector range $Q < 1$ 1/Å, the coherent signal in H2O is enhanced compared to the expectation for rigid, noninteracting, randomly oriented molecules. Since this Q-range corresponds to distances of several molecular spacings, our results provide evidence that intermolecular correlations in water extend beyond short-range correlations and involve more distant neighbors, giving rise to cooperative dynamical fluctuations. Such an enhancement can be rationalized by correlated preferential molecular orientations, hydrogen-bond rearrangements, and nuclear quantum effects. In contrast, D2O follows a more hydrodynamic behavior consistent with reported differences in the molecular bonding and symmetry of H2O and D2O. [1] M. Russina et al., J. Phys. Chem. Lett. (2025).

CPP 35: Glasses and Glass Transition (joint session DY/CPP)

Time: Wednesday 11:15–12:45 Location: ZEU/0118

Invited Talk CPP 35.1 Wed 11:15 ZEU/0118

Topological defects in 2D amorphous ensembles — •Peter Keim — Heinrich-Heine-Universität Düsseldorf

Topological defects are key to understand melting of crystals in two dimensions. A dilute gas of bound thus virtual pairs of dislocations cause the softening of a crystal in the vicinity of melting. If thermal energy is high enough to unbind dislocation pairs, translational order is destroyed and the crystal to melts due to the lack of shear resistance. In an amorphous solid, the concept of topology seems useless for the first glance due to the absence of order. Here, we discuss, how the definition of virtual dislocations can be generalized for a two-dimensional glass. Based on positional data of a binary colloidal monolayer we determine the fugazity of generalized virtual dislocations and measure elasticity close to the glass transition: Youngs modulus gets 16π at melting in surprisingly close analogy to Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) - theory for melting of 2D crystals.

CPP 35.2 Wed 11:45 ZEU/0118

Glass transition and universal scaling in ultra-low crosslinked microgels — Alessandro Martinelli[1], Rajam Elancheliyan[1], Andrea Scotti[2], Alexander V. Petrunin[3], •Domenico Truzzolillo[1], and Luca Cipelletti[1,4] — [1]Laboratoire Charles Coulomb (L2C), UMR 5221 CNRS-Universitè de Montpellier, F-34095 Montpellier,France — [2]Division of Physical Chemistry, Lund University, SE-22100 Lund, Sweden — [3]Institute of Physical Chemistry, RWTH Aachen University, Landoltweg 2, 52074 Aachen,Germany — [4]Institut Universitaire de France, F-75231 Paris, France

We investigate the glassy dynamics of Ultra-Low Crosslinked (ULC) poly(N-isopropylacrylamide) (PNIPAM) microgels. The glass transition is reached by varying either the temperature (modulating microgel swelling) or the colloidal number density. Our Dynamic Light Scattering (DLS) measurements confirm that the dynamic slowdown is solely governed by the effective volume fraction (φ), with ULC microgels behaving as fragile glass formers. Small-Angle X-ray Scattering data further indicates that the center-to-center inter-microgel distance is insensitive to temperature, scaling geometrically with mass fraction, while the height of the first peak of the static structure factor decreases with increasing concentration, suggesting structural melting above glass transition. We finally we report on the striking emergence of a universal dynamic behavior for the relaxation time (τ_α) dependence on the scattering vector (q) across the entire supercooled and glass regimes, allowing the data to collapse onto a master curve, whose features will be discussed.

CPP 35.3 Wed 12:00 ZEU/0118

Strain-rate dependent rheological memory in a model glass former — •Monoj Adhikari and Jürgen Horbach — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany

We investigate the shear response of deeply supercooled liquids far below the mode coupling critical temperature of a model glass former. Our system is based on the Kob-Andersen binary Lennard-Jones mixture (KABLJM) model but incorporates polydispersity, allowing us to combine SWAP Monte Carlo (MC) with Molecular Dynamics (MD) simulations. This hybrid approach enables equilibration at temperatures far below the Mode-Coupling critical temperature, T_{MCT}, while maintaining an equation of state similar to the original binary KABLJM model. We examine the response of these equilibrated samples to shear deformation at finite temperature and strain rate. By combining MD with SWAP MC during shear, we demonstrate that states with stress far below the yield stress can be accessed, making Newtonian fluid behavior observable even at temperatures well below T_{MCT}. To characterize the Newtonian fluid states obtained from this hybrid approach, as well as the solid-like states from standard MD, we employ a strain-rate switching protocol on the steady states. When applying this protocol to the stationary states, we observe intriguing memory effects. In the transient regime, stress overshoots appear when increasing the strain rate, whereas a striking stress undershoot emerges when decreasing it, mirroring recent experimental observations in polymer glasses.

CPP 35.4 Wed 12:15 ZEU/0118

An Analytical Relation between Thermodynamics and Dynamics in a Trap-like Model of Supercooled Liquids — •Simon G. Kellers, Anshul D. S. Parmar, and Andreas Heuer — Institute of Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster, Germany

Recent studies on 2D non-network glass formers, enabled by the million-fold acceleration of Swap Monte Carlo, have revealed clear deviations from Gaussian behavior in the inherent-structure (IS) density of states and linked these features to the fragile-to-strong crossover (FSC) and the emergence of a low-energy depletion regime.

Here, we establish such a connection by introducing a direct analytical relation between thermodynamic PEL statistics and dynamical properties within a trap-like description of supercooled liquids. We illustrate this relation using a binomial distribution of IS states and show that it naturally yields a characteristic trap size for polydisperse systems. This trap size reflects the effective number of degrees of freedom that collectively determine the depth and barrier of a metabasin participating in an activated relaxation event, thereby offering a physically transparent measure of cooperativity.

By combining this analytical framework with simulation data for a polydisperse 2D glass former, we obtain a coherent and quantitatively consistent landscape-based interpretation of the FSC.

[1] Andreas Heuer, J. Condens. Matter Phys. 2008, 20, 373101

[2] Anshul D. S. Parmar, Andreas Heuer, 2023 arXiv preprint arXiv:2307.10143

CPP 35.5 Wed 12:30 ZEU/0118

Single particle vs. collective diffusion dynamics in a glass-forming ternary Lennard-Jones mixture — •Anna Pini and Jürgen Horbach — Institut für Theoretische Physik II: Soft Matter, Heinrich Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf

Ternary fluid mixtures exhibit a rather complicated diffusion dynamics compared to their binary counterparts. Apart from three self-diffusion coefficient, there are three interdiffusion coefficients. In this work, we study a ternary ABC Lennard-Jones mixture using molecular dynamics computer simulation. It is based on the Kob Andersen binary Lennard-Jones mixture (KABLJM) [1] to which we have added a third C component. While C-C and A-C interactions are respectively identical to A-A and A-B interactions, B-C interactions are different from those between A and B particles. We study the glassy dynamics of this system at a high density of $\rho = 1.2$ and compare it to that of the original KABLM. While the self-diffusion coefficient show a similar temperature dependence for the binary and the ternary system, the behavior of the interdiffusion coefficients in the ternary system is significantly different from that in the binary one; in particular, unlike the binary system, the Darken equation does not hold in the ternary one. [1] W. Kob and H. C. Andersen, Phys. Rev. Lett. **73**, 1376 (1994).

CPP 36: Round Table Discussion: The Future of Neutrons in France and Germany (joint session CPP/BP)

Organized by Benoit Coasne and Christine M. Papadakis.

Time: Wednesday 11:45–12:45 Location: ZEU/LICH

Discussion CPP 36.1 Wed 11:45 ZEU/LICH

Round Table: Novel Opportunities for France/Germany Cooperation in Neutron Science — •Julian Oberdisse[1], •Frank Schreiber[2], •Arnaud Desmedt[3], •Stephan Förster[4], •Jacques Jestin[5], •Pascale Launois[6], •Christian Pfleiderer[7], and •Sabrina Disch[8] — [1]Laboratoire Charles Coulomb, U Montpellier, France — [2]Institut für Angewandte Physik, Universität Tübingen, Germany — [3]Laboratoire Léon Brillouin (LLB), Gif-sur-Yvette, France, — [4]Jülich Centre for Neutron Science (JCNS), FZ Jülich, Germany — [5]Institut Laue-Langevin (ILL), Grenoble — [6]Laboratoire de Physique des Solides d'Orsay, France — [7]Heinz Maier-Leibnitz Zentrum (MLZ), Garching, German — [8]University of Duisburg-Essen, Germany

With current and upcoming major changes in European neutron science and facilities, Germany and France are expected to play a strong role. This emerging new landscape for neutron science offers opportunities to reshape and reinvent the traditionally strong bonds between our two countries – both in terms of science cooperation and technical collaboration. The hosts Julian Oberdisse and Frank Schreiber look forward to a diverse panel discussion with the directors of the French and German neutron facilities as well as the chairs of the French and German neutron associations.

CPP 37: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics III

Time: Wednesday 15:00–16:45 Location: ZEU/LICH

Invited Talk CPP 37.1 Wed 15:00 ZEU/LICH

Predicting molecular ordering in deposited molecular films — •Denis Adrienko — Max Planck Institute for Polymer Research, Mainz, Germany

Thin films of molecular materials are commonly employed in organic light-emitting diodes, field-effect transistors, and solar cells. The morphology of these organic films is shown to depend heavily on the processing used during manufacturing, such as vapor co-deposition. However, the prediction of processing-dependent morphologies has until now posed a significant challenge, particularly in cases where self-assembly and ordering are involved. In this work, a method is developed based on coarse-graining that is capable of predicting molecular ordering in vapor-deposited films of organic materials. The method is tested on an extensive database of novel and known organic semiconductors. A good agreement between the anisotropy of the refractive indices of the simulated and experimental vapor-deposited films suggests that the method is quantitative and can predict the molecular orientations in organic films at an atomistic resolution [1]. The methodology can be readily utilized for screening materials for organic light-emitting diodes.

[1] C. Scherer, N. Kinaret, K.-H. Lin, M. N. Qaisrani, F. Post, F. May, D. Andrienko, Adv. Energy Mater., 14, 2403124, 2024

CPP 37.2 Wed 15:30 ZEU/LICH

A Universal Soft Upper Limit to the Seebeck Coefficient in Organic Thermoelectrics — •Dorothea Scheunemann[1], Zelong Li[2], Dennis Derewjanko[1], Yuqian Liu[2], Martijn Kemerink[1], and Guangzheng Zuo[2] — [1]Heidelberg University, Germany — [2]Fudan University, Shanghai, P.R. China

Organic thermoelectrics have the potential to convert waste heat into electricity by utilizing lightweight and flexible polymers. Despite over a decade of intensive research, significant progress remains limited. A key factor is the trade-off between conductivity (σ) and Seebeck coefficient (S), which dictates the extent to which the power factor ($PF = \sigma S^2$) can be optimized. Here, we combine an experimental data set for different polymers at variable doping levels to show that the S vs. σ curve is universal up to the maximum PF, followed by a material-dependent roll-off, when S and σ are normalized to their values at maximum PF. Furthermore, it is demonstrated that there is a soft upper limit for S ($\sim$200μV/K), at which the optimal power factor is achieved. Combining tight-binding and kinetic Monte-Carlo modeling, we quantitatively explain this behavior in terms of quasi-free charges moving in a renormalized density of states of Gaussian shape, where the renormalization accounts for the screened interaction with the ionized dopants. These findings suggest that the trade-off only exists at the single-material level, which subsequently gives rise to practical design rules.

CPP 37.3 Wed 15:45 ZEU/LICH

Nanoscale Dry-Processed Phosphorescent Films for Programmable Photonic Applications — •Yana Bui Thi, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden

Room-temperature phosphorescence (RTP) of organic materials provides a versatile basis for applications in environmental detection, security features, and optical data storage. Many of these concepts, including programmable luminescent tags (PLTs) [1], rely on precise control of triplet states, which poses certain challenges in terms of stability and processing. While polymer matrices are commonly used to suppress non-radiative decay, their processing limitations have restricted the miniaturization and control of devices. Here, we introduce ultrathin RTP tags that are produced entirely solvent-free and use organic materials as active layer. These nm-sized stacks exhibit higher efficiency and can be more than twenty times thinner than polymer-based structures. We characterize the resulting activation dynamics, stability, and reusability and discuss how the processing enables improved uniformity and the possible integration with structuring techniques. These results demonstrate a path toward compact, low-energy, and precisely controllable luminescent tags for future photonic technologies.

[1] Gmelch et.al. High-Speed and Continuous-Wave Programmable Luminescent Tags Based on Exclusive Room Temperature Phosphorescence (RTP). Adv Sci. 2021 (23):e2102104.

CPP 37.4 Wed 16:00 ZEU/LICH

Probing the percolating charge transport network in organic semiconductors by noise spectroscopy — •Sebastian Klein, Priya Viji, Constantin Tormann, Clemens Göhler, and Martijn Kemerink — IMSEAM, Heidelberg University, Germany

In disordered organic semiconductors (OSCs), a suppression of shot noise is expected due to the internal charge carrier transport mechanisms, which is relevant for, e.g., their application in photodetectors. The charge transport in OSCs, which occurs by hopping between localized sites, can be described by percolation theory, from which it follows that so-called hard hops form the bottleneck that charge carriers have to overcome to progress through the device. The tunneling through one singular hard hop is a random uncorrelated poissonian process which leads to OSCs displaying shot noise. Since multiple hard hops sit in series in the charge transport path in macroscopic OSCs, it is expected that shot noise in OSC is suppressed, inversely proportional to the number of hard hops, which in turn depends on disorder, temperature and thickness of the OSC. This suppression is quantified by the Fano factor, which we directly measure by current cross-correlation noise spectroscopy. Temperature- and current-bias-dependent Fano factor measurement results are compared with kinetic Monte Carlo simulations. From the measurements and simulations, it can consistently be concluded that Fano factor measurements give direct and otherwise inaccessible insight into the internal structure as well as the disorder and correlation length of OSC.

CPP 37.5 Wed 16:15 ZEU/LICH

Charge transfer dynamics in PBDB-T blends studied by time-resolved optical spectroscopy — Beatriz Molinaro Guerra[1], Federico Cilento[2], Maria Luiza Miranda Rocco[1], and •Wibke Bronsch[2] — [1]Institute of Chemistry, Federal University of Rio de Janeiro, 21941-909, Rio de Janeiro-RJ, Brazil — [2]Elettra-Sincrotrone Trieste S.C.p.A., 34149 Basovizza, Trieste, Italy

Charge transport processes in conjugated polymers are an important key for the production of more efficient organic optoelectronic devices, such as organic solar cells. Specially, the study of electron charge transfer dynamics in excited states may help us to understand charge transport properties in these materials. We studied the ultrafast response of different blends of PBDB-T polymers with small molecules after NIR excitation. Time-resolved optical spectroscopy measurements with broad-band probe pulses performed in the T-ReX facility at Elettra reveal clear changes in the ultrafast response when comparing the results for the pure molecule films and the blends, suggesting that charges are transferred between the two components of the blend on the femto- to picosecond timescale. After exciting the HOMO-LUMO transition of the ITIC molecule, the exciton population decay time drastically reduces due to the presence of the PBDB-T polymer, while the decay constant at photon energies in the range corresponding to the PBDB-T HOMO-1-LUMO transition increases. This behavior indicates hole injections in PBDB-T after primary excitation of ITIC, as it was also discussed for PBBF:ITIC blends [1]. [1] Liu et al. Advanced Science 6, 1802103 (2019).

CPP 37.6 Wed 16:30 ZEU/LICH

Analysis of Charge Carrier Dynamics in Organic Solar Cells via Optical Impedance Spectroscopy — •Elias Wassmer, Jan Phillip Ott, Brian Hinz, Clemens Göhler, and Martijn Kemerink — IMSEAM, Heidelberg University, Germany

Understanding the complex dynamics of charge carriers in organic solar cells (OSCs) is essential to identify the mechanisms that lead to voltage, current and fill factor losses. In this work, we investigate these dynamics by combining conventional electrical impedance spectroscopy (EIS) with the newly implemented optical impedance spectroscopy (OIS). In OIS, in addition to a constant background illumination, a small alternating light signal is applied to investigate the photogenerated charge carriers under quasi-steady-state conditions. The results of both EIS and OIS of PM6:Y6 OSCs across a range of operating conditions are used to compare the two methods and allow us to track changes during device degradation. To interpret the measured impedance spectra, two established models are applied: an equivalent-circuit model, which maps the behaviour of the OSC onto a network of resistances and capacitances, and a rate-equation model that describes carrier generation, recombination and extraction through differential equations. Comparing these modelling approaches allows us to evaluate how well the charge-carrier dynamics are captured by each model and how this relates to the physical processes inside the OSCs. Our results show that the equivalent-circuit model is insufficient for describing OIS, indicating that a more physically motivated rate-equation model is needed to reproduce photogenerated carrier dynamics.

CPP 38: Biopolymers, Biomaterials and Bioinspired Functional Materials I (joint session CPP/BP)

Time: Wednesday 15:00–16:45 Location: ZEU/0255

Invited Talk CPP 38.1 Wed 15:00 ZEU/0255

Engineering, processing and application of recombinant spider silk proteins — •Thomas Scheibel — Universität Bayreuth, Lehrstuhl Biomaterialien, Prof.-Rüdiger-Bormann-Str. 1, 95440 Bayreuth

Proteins reflect one fascinating class of natural polymers with huge potential for technical as well as biomedical applications. One well-known example is spider silk, a protein fiber with excellent mechanical properties such as strength and toughness. We have developed biotechnological methods using bacteria as production hosts which produce structural proteins mimicking the natural ones. We employ silk proteins in application forms such as fibers, hydrogels, particles or films with tailored properties, which can be employed especially for biomaterials applications. In case of implants or catheters cell adhesion plays a crucial role for the overall function of the to-be-used material. To change the properties of in-use polymers and to adopt their biocompatibility, we established coatings based on engineered spider silk proteins. Spider silk hydrogels can be employed as new bioinks for biofabrication. Their elastic behavior dominates over the viscous behavior over the whole angular frequency range with a low viscosity flow behavior and good form stability. Cell-loaded spider silk constructs can be easily printed without the need of additional cross-linkers or thickeners for mechanical stabilization. Our bio-inspired approach serves as a basis for new materials in a variety of medical, biological, or technical applications.

CPP 38.2 Wed 15:30 ZEU/0255

Inferring Structure-Property Relationships with Artificial Intelligence: A Lignin Case Study — •Matthias Stosiek and Patrick Rinke — Department of Physics, Atomistic Modelling Center, Munich Data Science Institute, Technical University of Munich

The potential of lignin as an abundant, underutilized biopolymer is increasingly being realized. A key challenge for the targeted production of lignins remains the poorly understood relation between lignin properties and its complex structure. Artificial intelligence (AI) methods could reveal such structure-function relationships but remain elusive in biomaterials research.

95 structurally diverse lignins are extracted from birch wood combining the Aqua Solv Omni (AqSO) biorefinery process and AI-guided data acquisition [1, 2]. Each lignin sample is characterized with 2D NMR spectroscopy and complemented with measurements of key lignin properties such as antioxidant activity.

To establish structure-function relationships, we correlate regions of the NMR spectra with corresponding property measurements. With a feature importance analysis, we identify structural relevant features for each property and provide a chemical interpretation. For instance, we find that more β-O-4 bonds lead to lower surface tension in water indicating a more linear lignin structure. Our structure-inference approach is designed to be general and applicable to a wide range of materials and characterization data.

[1] D. Diment et al., ChemSusChem, e202401711 (2024). [2] M. Alopaeus, M. Stosiek et al., Sci Data 12, 996 (2025).

CPP 38.3 Wed 15:45 ZEU/0255

A minimalist view on biopolymer phase separation and aging — •Jasper Michels — Max Planck Institute for Polymer Research, Mainz, Germany

Phase separation of proteins is a ubiquitous process by which cells regulate biological processes. In aberrant cases, such as encountered in neurodegeneration, initially liquid condensates age to become more solid-like. Understanding the interplay between phase separation and aging seems essential in the development of new therapeutic strategies. We apply minimal models that aim to capture the essence of biological transitions in terms of driving forces and thermodynamics. Models discriminating between mono- and multivalent directed association on the one hand and non-specific interactions on the other appear surprisingly versatile in reproducing and predicting biopolymer phase behavior, while at the same time providing essential mechanistic insight. We will review our efforts, combining theory with experiments and demonstrating how relatively simple descriptions can (re)produce complex multi-component phase behavior. We will also present a dynamic version of the model, which provides for a thermodynamically fully consistent and intuitive description of the experimentally observed changes in viscoelasticity during aging. Our calculations explain how the stickiness of the proteins changes with time and concentration and how the coupling between association and solvation determines condensate viscoelasticity.

CPP 38.4 Wed 16:00 ZEU/0255

Cellulose-colloid hybrid materials for refractive index tuning — •Stephan V. Roth — Deutsches Elektronen-Synchrotron DESY, Hamburg, Sweden — KTH Royal Institute of Technology, Stockholm, Sweden

Cellulose nanofibrils (CNF) with tailored (negative) surface charge are ideal for stable, nanoporous, structure-guiding network for thin film composite materials. Colloid materials offer the possibility for tunable structural colors, templates for metamaterials, and refractive index tuning. Here, core-shell-colloids with a hydrophobic core and positively charged, hydrophilic shell are used as additive in CNF thin films to tune their refractive index. The imbibition and self-assembly of the colloids as a function of colloid diameter in the CNF network was quantified, with colloids smaller than the pores in the CNF network penetrating into the thin film. Subsequent heat treatment allows for nanoscale composite formation on the level of the ~ 10 nm sized CNF bundles, while humidity treatment homogenizes the colloid distribution. Furthermore, the influence of the colloid size on the CNF structure inside the thin film was investigated and related to the mechanical properties of the colloid-CNF composite.

CPP 38.5 Wed 16:15 ZEU/0255

A universal material basis for biocompatible printed electrolytes in Organic Electrochemical Transistors (OECTs) — •Moritz Flemming, Paul Zechel, Rakesh Nair, Laura Teuerle, Hans Kleemann, and Karl Leo — Institute of Applied Physics, Technische Universität Dresden

Organic Electrochemical Transistors (OECTs) stand out for their interplay between ionic and electronic conduction, making them ideal analogues to biological synapses for neuromorphic computing or biosensors. Furthermore, they can be printed into integrated circuits on flexible substrates, allowing for low-cost and high throughput fabrication of full electronic systems. However, most OECT electrolytes for integrated circuits still lack biocompatibility and suffer from rheology-related printing challenges. This talk presents a novel material basis that can be combined with an ionic liquid to fabricate a biocompatible electrolyte for OECTs. It allows rheological adjustments to enable the use of electrolyte in both inkjet and screen printing. Furthermore, the electrolyte is UV-curable, enabling it to transition into solid-state structures after printing. Extended ink and device lifetimes for screen-printed structures enable the fabrication of state-of-the-art OECTs that can operate in ambient air more than 30 days after fabrication. Ultimately, a fully biocompatible and screen-printed OECT on a leaf substrate is demonstrated.

CPP 38.6 Wed 16:30 ZEU/0255

Nonequilibrium dynamics of the helix-coil transition in polyalanine — •Maximilian Conradi[1], Fabio Müller[1], Suman

Majumder[2], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany — [2]Amity Institute of Applied Sciences, Amity University Uttar Pradesh, Noida 201313, India

As a continuation of our previous work, the nonequilibrium pathways of the collapse of the helix-forming biopolymer polyalanine are investigated in an explicit solvent. To this end, the full time evolution of the helix-coil transition is simulated using molecular dynamics simulations. We compare the phenomenology of the transition between the two studies and investigate the dynamics.

CPP 39: French-German Session: Nanomaterials, Composites and Hybrids I

Time: Wednesday 15:00–16:45 Location: ZEU/0260

Invited Talk CPP 39.1 Wed 15:00 ZEU/0260

A polarizable model for atomistic simulations of metals and graphitic material/ liquid interfaces — Krishan Kanhaiya[1], Hendrik Heinz[2], and •Marialore Sulpizi[1] — [1]Department of Physics and Astronomy, Ruhr-University Bochum, Universitätsstraße 150, 44801 Bochum, Germany — [2]Department of Chemical and Biological Engineering, University of Colorado at Boulder, Boulder, CO 80301

Polarization significantly affects the interaction and adsorption energy of molecules on metal surfaces. The ability to describe at a metal surface the classical "image charge" potential is a direct result of its polarizability, which needs to be modelled correctly to accurately simulate interfacial phenomena e.g. in electrochemistry or catalysis. Recently, we have introduced a polarizable model for metals which permits to describe also electrified interfaces. Here we extend the idea to graphitic material introducing flexible dummy electrons to represent the polarizable π-electron cloud. The model accurately predicts surface and hydration energy, water contact angle as well as experimental and DFT data on molecular adsorption on surfaces. A considerable improvement is obtained in the prediction of water-graphite interfacial friction, which is obtained at the level of electronic structure calculations.

CPP 39.2 Wed 15:30 ZEU/0260

Lamellar Domain Spacing of Copolymers with Nonlinear Block Architectures — Andrzej Grzyb[1], Jarosław S. Kłos[2], Aykut Erbaş[3], Michael Lang[4], and •Jarosław Paturej[1] — [1]Institute of Physics, University of Silesia, Katowice, Poland — [2]Faculty of Physics, A. Mickiewicz University, Poznań, Poland — [3]UNAM, Bilkent University, Ankara, Turkey — [4]Leibniz-Institut für Polymerforschung Dresden e.V., Germany

Topological modification of block copolymer (BCP) conformations offers a promising approach for developing self-assembled periodic nanostructured materials with smaller domain sizes, which are essential for a range of technological applications. Cyclic polymers, with their inherently more compact conformations, present an effective strategy for achieving this miniaturization. In this work, through a combination of analytical theory and coarse-grained molecular dynamics simulations, we establish a relationship between different nonlinear topologies and the corresponding domain size of lamella-forming BCPs. Our investigations includes BCP architectures with one or two cyclic segments such as tadpoles, diblock and triblock 8-shaped polymers, and diblock nonconcatenated and concatenated rings. We demonstrate that the primary reduction in lamellar domain size is driven by the more compact arrangement of monomers in the cyclic architectures, with an additional contribution from the nonconcatenation of cyclic segments. This is corroborated by theoretical predictions for both domain size reduction and BCP conformations across different architectures.

CPP 39.3 Wed 15:45 ZEU/0260

Self-Healing Composite Structures for Aerospace Applications — •Merve Ozkutlu Demirel[1], Eray Kostur[1,2], Yigitalp Okumus[1], Bilal Altin[1], Melih Seckin[1], and Yahya Oz[1] — [1]Turkish Aerospace, R&D and Advanced Technologies Directorate, 06980 Ankara, Turkiye — [2]Cukurova University, Department of Mechanical Engineering, 01330 Adana, Turkiye

Self-healing composite structures offer a promising solution for enhancing durability and reducing maintenance costs in aerospace platforms. In this study, a self-healing mechanism based on a microvascular channel network was developed. Composite laminates were fabricated using carbon fabric and epoxy resin. Polyamide monofilaments with a diameter of 450 um were integrated into a hand lay-up process by placing them between composite layers. After curing, these fibers were removed to create hollow channels. Various channel configurations were manufactured and evaluated through bending tests. 5-Ethylidene-2-norbornene was selected as healing agent because its operating temperature range is similar to flight temperature conditions. The healing agent was injected into the channels, while the Grubbs catalyst that would start the polymerization reaction was uniformly dispersed within the polymer matrix. Upon crack formation, the healing agent is expected to flow into the damaged region and polymerize upon contact with the catalyst, thereby filling the crack. Compact tension tests were performed to analyse the healing performance. The results demonstrated that the microvascular channel approach exhibits strong potential for aerospace applications.

CPP 39.4 Wed 16:00 ZEU/0260

Increasing the Mechanical Stability of Carbon Nanomembranes Using a Holey Carbon Interlayer — •Luzie Lina Heinrichs, Zhen Yao, Yang Yang, and Armin Gölzhäuser — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

Carbon nanomembranes (CNMs) are atomically thin, with subnanometre pores that enable strong gas selectivity and fast, efficient water transport. However, their limited mechanical robustness has constrained their integration into practical filtration technologies.

In this study, we introduce a reinforced CNM architecture that incorporates an intermediate holey support layer. We fabricate and compare single-layer, double-layer, and holey film reinforced composite CNMs. Water permeation measurements using a cup test, combined with nanoindentation characterisation, show that the reinforced architecture preserves high water permeability while markedly improving mechanical stability. The effective Young's modulus reaches ~25 GPa, approximately five times higher than that of an unreinforced double layer.

By combining mechanical robustness with efficient single-file water transport and precise selectivity, the holey-layer-reinforced CNMs provide a promising route toward real-world applications, especially in seawater desalination.

CPP 39.5 Wed 16:15 ZEU/0260

Particle distribution and thermoresponsive properties of PNIPAM brush/gold nanoparticle composite films — •Elias Hallenbach, Marvin Glock, Hayden Robertson, and Regine von Klitzing — TU Darmstadt, Institute for Condensed Matter Physics, 64289 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.

Polymer brushes can 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 grafting density [1]. Nanoparticle uptake has proven to be highest at intermediate grafting densities [2]. In the present study thermoresponsive Poly(N-Isopropylacrylamide) brushes with varying grafting densities were synthesized directly from a silicon substrate. Nanocomposite materials were fabricated by dip-coating of polymer brushes into an AuNP suspension. Characterization of nanocomposites was performed by (in situ) spectroscopic ellipsometry, atomic force microscopy and (in situ) X-ray reflectometry. The relation between particle distribution and temperature-induced structural changes will be discussed.

[1] S. Christau et al., *Polymers* **2014**, *6*, 1877-1896.

[2] R.R. Bhat, J. Genzer, *Appl. Surf. Sci.* **2006**, *252*, 2549-2554.

CPP 39.6 Wed 16:30 ZEU/0260

Morphology-controlled electrical and thermal conductivity of filled diblock copolymers: effect of filler shape. — •Alexander

Chervanyov — University of Münster, Münster, Germany

We investigate the electrical and thermal conductivity of an electrically insulating diblock copolymer (DBC) matrix filled with conductive cylindrical and spherical nanofillers modeling carbon nanotubes (CNTs) and carbon black (CB), respectively. The composite transport properties are examined as functions of the underlying DBC morphology, the selective affinities of CNTs and CB for the dissimilar DBC blocks, and inter-filler interactions that determine the positional and, for CNTs, orientational correlations. Using a combined phase-field description of the DBC host and Monte Carlo simulations of anisotropic CNT fillers, we show that the localization and alignment of CNTs within the microphase-separated domains are highly sensitive to the above parameters. The simulated CNT and CB network structures are used to compute the electrical and thermal response of the composite. We quantitatively elucidate how the morphological transitions in the DBC correlate with structural rearrangements of the filler networks. Furthermore, we demonstrate that both the order-disorder transition and the order-order transitions between distinct DBC morphologies lead to pronounced changes in composite conductivity, driven by morphology-induced restructuring and alignment of the conductive pathways formed by CNT and CB.

Financial support of Deutsche Forschungsgemeinschaft (DFG) through Grant No. CH 845/2-3, is gratefully acknowledged.

CPP 40: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics IV

Time: Wednesday 17:00–18:30 Location: ZEU/LICH

CPP 40.1 Wed 17:00 ZEU/LICH

Morphological Disorder Boosts Charge Separation in Single-Component OPDs — •Michel Panhans[1], Jakob Wolansky[2,3], Karl Leo[2], Johannes Benduhn[2,3], and Frank Ortmann[1] — [1]TUM School of Natural Sciences and Atomistic Modeling Center, Munich Data Science Institute, Technische Universität München, 85748 Garching b. München, Germany — [2]Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, 01069 Dresden, Germany — [3]DZA, Görlitz, Germany

Single-component organic photodetectors (OPDs) provide a simplified alternative to donor-acceptor heterojunctions, yet their operation mechanisms remain theoretically underexplored. We investigate the molecular origin of charge generation in vapor-deposited DCV2-5T by modeling the excitonic density of states with an effective exciton Hamiltonian that incorporates electronic coupling, Coulomb interaction, and structural disorder. Disorder is introduced through lateral shifts between π-stacked molecules, which notably modulates electronic and excitonic couplings. Simulations show that intermediate disorder reproduces the experimental external quantum efficiency, while strong disorder enhances hybridization between excitonic states. This hybridization enables exciton delocalization via a superexchange-like mechanism, increasing the probability of charge separation. Counterintuitively, disordered domains exhibit stronger coupling than crystalline ones, suggesting that reduced structural order can facilitate charge generation. These insights highlight morphology-dependent excitonic interactions as a design principle for self-driven OPDs.

CPP 40.2 Wed 17:15 ZEU/LICH

Limiting factors to free charge generation in low-bandgap organic blends for photovoltaic applications and beyond — •Manasi Pranav[1], Atul Shukla[1,2], and Dieter Neher[1] — [1]University of Potsdam, Potsdam, Germany — [2]University of Queensland, Brisbane, Australia

Despite possessing similar theoretical limits, state-of-the-art organic solar cells outshine low-bandgap organic blends (absorption edge beyond 1000 nm) in their exciton harvesting efficiency. An understanding of these free charge generation mechanisms is needed to tap into the potential of such low-bandgap non-fullerene acceptors (NFAs) for photovoltaic and photodetector applications. To this end, we probe the pathways of exciton dissociation and charge-transfer state separation in multiple D:NFA systems with varying absorption edges, and varying extents of energy-transfer or charge-transfer prior to free charge generation. This is done by combining transient and steady-state optoelectronic techniques, to resolve the losses incurred between photon absorption and carrier extraction. For some of these systems, namely in blends using Y6 derivatives with extended pi-conjugation, we find that the kinetic competition between geminate charge-transfer state decay and its separation is a major limiting role in the overall photon harvesting capability of the devices. As part of ongoing work, these investigations aim to reveal the underlying geminate loss pathways, which limit overall internal quantum efficiency of the blends and, in turn, limit the figures of merit of the resulting devices.

CPP 40.3 Wed 17:30 ZEU/LICH

Consistency of Electron-Vibrational Coupling Across Methods? A Comparative Study — •Maximilian F. X. Dorfner, Konrand Merkel, and Frank Ortmann — Department of Chemistry, TUM School of Natural Sciences, and Atomistic Modeling Center, Munich Data Science Institute, Technical University of Munich, München, Germany

Characterizing electron-vibrational interaction in materials is a nontrivial theoretical task, owing to the differing definitions of coupling constants and the variety of available methods for computing these. This diversity naturally raises questions about the consistency and reliability of the methods used and their interrelation.

To address this issue, this contribution presents a systematic comparison of electron-vibrational coupling calculations. We summarize our findings on the relationship between density functional theory approaches and quasi-particle methods [1], study the influence of different exchange and correlation functionals, and investigate the impact of various ab initio methodologies [2] on the resulting electron-vibrational coupling constants.

Our findings provide guidelines and data for validating methodologies and estimating theoretical errors in coupling constant calculations.

[1] M.F.X. Dorfner and F. Ortmann, J. Chem. Theory Comput. 2025, 21, 5, 2371-2385; [2] K. Merkel, M.F.X. Dorfner and F. Ortmann, J. Phys. Mater. 8 045014

CPP 40.4 Wed 17:45 ZEU/LICH

Enhanced Photo-multiplication Effect through Synergistic Hole Blocking and Traps Engineering in OPDs — •Awais Sarwar[1], Louis Conrad Winkler[1,2], Karl Leo[1], and Johannes Benduhn[1,2] — [1]IAPP, TU Dresden, Germany — [2]DZA, Görlitz, Germany

Photomultiplication-type organic photodetectors (PM-OPDs) are highly effective for detecting weak light. However, they often face a significant trade-off: high gain usually results in excessive noise and slow response times. To overcome these limitations, we introduce a vacuum-deposited broadband photodetector architecture that utilizes the synergistic integration of hole-blocking layers and precise traps engineering. By strategically controlling the charge injection barriers and trap distribution, this design effectively separates the gain mechanism from the noise floor. The resulting device achieves a peak external quantum efficiency (EQE) exceeding 1100 per cent, while maintaining a specific detectivity of 4.4*10e12 Jones at a bias of -2 V. Unlike slow trap-dominated systems, our optimised architecture keeps a cutoff above 25 kHz. Vacuum-deposited PM-OPDs offer high sensitivity and fast response, ideal for real-time sensing.

CPP 40.5 Wed 18:00 ZEU/LICH

Wavelength-dependent charge carrier extraction of organic solar cells under operational conditions — •Lara Bartnick, Martijn Kemerink, and Clemens Göhler — IMSEAM, Heidelberg University, Germany

Organic solar cells (OSCs) have recently achieved power-conversion efficiencies of about 20%, making them increasingly promising for renewable energy applications despite still falling behind silicon photovoltaics. To understand the mechanisms that limit their performance, highly sensitive external quantum efficiency (EQE) measurements are essential, as they show how efficiently photons of different energies generate extractable charge carriers across the UV- to near-infrared spectrum.

We have measured the EQE of current standard PM6:Y6 OSCs under different initial conditions including bias voltage in both reverse and forward direction, bias illumination, and temperature, to investigate how open-circuit voltage- and fill-factor losses can be attributed to wavelength-dependent charge carrier generation efficiencies. These measurements reveal that the spectral shape of the EQE is highly sensitive to biasing conditions. By relating the voltage dependent EQE to collection fields, we have been able to identify charge carrier extraction losses under typical working conditions, which are dependent on the incident photon energy. These findings, as well as wavelength- and voltage-dependent exciton generation and recombination rates, contribute to understanding the loss mechanisms and charge extraction behaviour of OSCs.

CPP 40.6 Wed 18:15 ZEU/LICH

Current Generation in Photomultiplication-type Organic Photodetectors — •Louis Conrad Winkler[1,2], Jonas Kublitski[1,3], Awais Sarwar[1], Hrisheekesh Thachoth Chandran[1], Wolfgang Tress[4], Urs Aeberhard[5], Karl Leo[1], and Johannes Benduhn[1,2] — [1]IAPP, TU Dresden, Germany — [2]DZA, Görlitz, Germany — [3]Departamento de Fisica, UTFPR, Curitiba, Brazil — [4]ZHAW, Winterthur, Switzerland — [5]FLUXiM, Winterthur, Switzerland

Organic photodetectors (OPDs) utilizing intrinsic gain promise enhanced performance in regard to faint light detection. While this gain mechanism boosts the external quantum efficiency (EQE), the associated noise often negates the net improvement of the specific detectivity D*. Nonetheless, the simplified readout circuitry and associated cost savings hold high potential for the market. Crucially, the origin of this photomultiplication (PM) effect is currently attributed to tunnel injection of charge carriers, driven by internal band bending due to trapped charge carriers. Here, we challenge this prevailing tunnel injection model based on comprehensive experimental evidence. We propose an alternative mechanism that offers a unified explanation for the gain observed across diode-like OPD architectures and validate it by drift-diffusion simulations. This model successfully provides general predictive capabilities regarding the magnitude and dependencies of the photocurrent gain. We rigorously tested this proposed mechanism across 29 diverse material systems, including both vacuum-processed and solution-processed devices.

CPP 41: Biopolymers, Biomaterials and Bioinspired Functional Materials II (joint session CPP/BP)

Time: Wednesday 17:00–18:45 Location: ZEU/0255

CPP 41.1 Wed 17:00 ZEU/0255

Coarse-grained simulations of network-forming DNA nanostructures — •Takahiro Yokoyama[1,2] and Arash Nikoubashman[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany

DNA nanotechnology offers exceptional nanoscale designability through precise control of DNA sequences. These individual DNA strands can form predetermined building blocks, which then hierarchically assemble into super-structures such as nanotubes, nanocapsules, or nanostars. The latter can assemble further into (percolated) networks, where sequence-level design enables systematic control of the rheological and mechanical network properties. This multi-scale self-assembly can lead to cascading effects, where even a single unpaired nucleotide on the building block level can act as a highly flexible hinge that dramatically alters the network mechanics. To understand how such variations on the nucleotide-scale affect the network properties, we designed a series of DNA networks by systematically altering the arm number and junction flexibility of the star-shaped building blocks using coarse-grained molecular simulations of the oxDNA model. Our study revealed that the bulk modulus of the network decreased with increasing number of DNA arms; this counter-intuitive behavior stems from the addition of flexible junctions on the single-star level, which preferentially absorb deformation and soften the overall network. This result highlights the importance of precise nanoscopic design on the order of one nucleotide to obtain optimal network properties.

CPP 41.2 Wed 17:15 ZEU/0255

Characterizing interactions between glycoproteins and RNA at the lipid membrane interface — •Horacio V. Guzman[1] and Viviana Monje[2] — [1]Biophysics & Intelligent Matter Lab, Material Science Institute of Barcelona, CSIC, Spain — [2]Department of Chemical and Biological Engineering, State University of New York at Buffalo, 308 Furnas Hall, Buffalo, USA

Biological membrane interfaces interacting with proteins, nucleic acids, and glycans are integral to many cellular processes. The interplay between membrane lipids and biopolymers is highly sensitive to their flexibility grade, secondary structure, and electrostatics. Consequently, the cell membrane interface experiences changes in local lipid distribution and fluctuation in local properties. Projecting biophysical and structural membrane and biopolymer properties onto a two-dimensional plane simplifies the quantification of molecular signatures by reducing the dimensional space and identifying relevant entropic and short-range interactions at the interface of interest, as well as, characterizing interaction patterns and spatial correlations of complex lipid bilayers as they interact with biopolymers. We compare lipid-lipid interaction patterns in membrane-only systems to the corresponding systems containing small proteins and RNA fragments, respectively. These analyses quantify the effect of peripheral biopolymers on local lipid composition, structure, packing, deformation ratio of the biopolymer, and surface topology of the membrane upon adsorption. Such characterization is crucial for starting with the next-generation rational design of lipid vesicles and lipid-coated RNA drug delivery systems.

CPP 41.3 Wed 17:30 ZEU/0255

Nanoscale characterization of piezoelectric nanofibers blended with Salmon Gelatin — •Martín Chavarría-Vidal[1], Dragica Bezjak[2], María Saavedra-Fredes[1], Benjamín Schleyer-Thiers[1], Ilka Hermes[3], and Tomás P. Corrales[1] — [1]Universidad Técnica Federico Santa María, Valparaíso, Chile — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Leibniz Institute of Polymer Research, Dresden, Germany

We electrospin salmon gelatin (SG) mixed in a polyvinyl alcohol (PVA) matrix containing chitosan (Ch). Furthermore, we used a coaxial electrospinning approach to blend these nanofibers together with polyvinylidene fluoride (PVDF). Such biomaterials could lead to the potential development of biocompatible and piezoelectric heart patches. After electrospinning our polymers, we observe by SEM two size distributions. Mechanical characterization of the large nanofibers obtained by AFM reveals two Youngs moduli peaks, centered at 1.77 GPa and 209 MPa. Small nanofibers also show a two component mechanical moduli distribution with peaks at 565 MPa and 1.33 GPa (10.1016/j.bbadva.2025.100168). EDS shows that both distributions contain Fluor. However, complimentary PFM measurements indicate that large nanofibers have a piezoelectric response comparable to pure electrospun PVDF, while the small ones do not exhibit such response. These measurements lead us to believe that the large nanofibers are mainly β-phase PVDF, while the smaller ones are composed of PVA/SG/Ch with α-phase PVDF (10.1177/15589250221125437).

CPP 41.4 Wed 17:45 ZEU/0255

Structural investigations using in situ SAXS on flexible bio-based vitrimeric carbon nanocomposites — •Sarathlal Koyiloth Vayalil[1,2], Vaishnav B[2], Viranchika Bijalwan[2], Saravendra Rana[2], and Ajay Gupta[2] — [1]Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — [2]Applied Science Cluster, UPES, Dehradun, India

In this work, in situ small- and ultra-small-angle X-ray scattering has been employed to investigate the real-time structural evolution of 3D-printed vitrimeric thiol-acrylate photopolymers and their carbon-based nanocomposites designed for healable strain-sensing and soft-robotic applications. Flexible bio-acrylate based vitrimers reinforced with graphene/CNT fillers at varying concentrations are examined to elucidate temperature-dependent phase segregation and enable direct visualization of nano- and microscale filler morphologies, their spatial distribution, and their evolution across key thermal transitions (Tg and Tv of the polymer matrix). The effects of the stress/strain and cyclic-thermal cycles on the filler aggregates affecting the composites conductivity in carbon-filled samples are also evaluated. These insights into nano- and microscale morphology, reinforcement, and conductive behavior help us understand the dynamic structure-property relationships governing vitrimer-based conductive networks

CPP 41.5 Wed 18:00 ZEU/0255

Nanomechanical testing of suspended single nanofibers and humidity-induced glass transition — •Benjamin Schleyer-Thiers[1], Diego Benavente[2], Yusser Olguin[2,3], and Tomas P. Corrales[1,3] — [1]Physics department of Universidad Tecnica Federico Santa Maria, Valparaiso, Chile — [2]Technological and Scientific Center (CCTVal), Valparaiso, Chile — [3]Biotechnology Center Daniel Alkalay Lowitt

In this work we will study the interaction of water molecules with polymeric nanofibers made from hygroscopic biopolymers and contrast them in environments with variable relative humidity. For this, we will suspend single nanofibers over micropatterns etched on silicon. In this suspended configuration, we shall perform three-point bending tests utilizing the environmental Atomic Force Microscope (AFM) and detect bending forces of the nanofiber, at different relative humidities. As bending tests are performed over the suspended nanofiber, the position-dependent stiffness can be plotted to find its mechanical modulus through bending models. The stiffness of single nanofibers drops with the increase in relative humidity, hinting a glass transition induced by this environmental condition. To test this behavior, we attempt to perform fracture experiments on a micro structured grid made by photolithography.

CPP 41.6 Wed 18:15 ZEU/0255

Probing light-induced drug release to lipid monolayers — •Ipsita Pani, Michael Hardt, and Björn Braunschweig — Institute of Physical Chemistry, University of Münster, Corrensstraße 28-30, Münster 48149, Germany

Light-induced drug release using photoresponsive nanocarriers is increasingly explored for targeted therapeutic applications. While most studies characterize release in bulk aqueous environments, drug release across aqueous-organic interfaces is equally important, as these interfaces represent the entry point into cells. We recently demonstrated light-induced drug release to air-water interface.[1] In cancer therapeutics, passive diffusion of anticancer drugs across lipid membranes is a key transport mechanism, yet direct quantitative data on drug-lipid interactions and their effect on release remain limited. Here, using arylazopyrazole photosurfactant nanocarriers and doxorubicin as a representative anticancer drug, we investigate how interfacial lipid composition governs light-induced drug release. By combining Langmuir monolayers with interface-specific vibrational sum frequency generation (SFG) spectroscopy, we quantitatively estimate drug release at lipid-adsorbed interfaces as a model membrane. To systematically probe headgroup effects, we employ four dimyristoyl lipids- DMPC, DMPG, DMPS, and DMPE which share identical acyl chains but differ in charge and polarity. These results elucidate how lipid-drug interactions modulate release efficiencies at membrane-like interfaces, providing insights key to the design of photoresponsive nanocarriers for targeted drug delivery. [1] Pani et al. Chem. Sci., 2024, 15, 18865-18871.

CPP 41.7 Wed 18:30 ZEU/0255

Hetero-aggregation of microplastic particles — Thomas Witzmann[1], Anja F. R. M. Ramsperger[2], Hao Liu[2], Yifan Lu[3], Holger Schmalz[2], Lucas Kurzweg[4], Tom C. D. Börner[4], Kathrin Harre[4], Andreas Greiner[2], Christian Laforsch[2], Holger Kress[2], Christina Bogner[3], Stephan Geckle[2], Andreas Fery[1], and •Günter K. Auernhammer[1] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Universität Bayreuth, Germany — [3]Universität zu Köln, Germany — [4]Hochschule für Technik und Wirtschaft Dresden, Dresden

Microplastic particles (MPP) in the environment are surrounded by a layer known as an 'eco-corona'. This is made up of natural organic matter (NOM), such as biomolecules, humic substances, and other natural molecules. NOM substantially alters the surface properties of MP particles, thereby influencing their interaction with other surfaces in an aqueous environment and their aggregation behaviour. We studied the interactions of eco-corona-covered MP particles on the nanoscale using colloidal probe-AFM. Measurements were performed at different ionic concentrations to mimic changing environmental conditions. We found that the eco-corona can pull on the silica colloidal probe via polymer bridging. This mechanism leads to aggregation and, consequently, sedimentation in the environment. By comparing our AFM results with experiments and simulations at different length scales, we consistently found that this type of heteroaggregation is conducive to stable aggregate formation and retains MPPs in sediments.

CPP 42: French-German Session: Nanomaterials, Composites and Hybrids II

Time: Wednesday 17:00–18:45 Location: ZEU/0260

Invited Talk CPP 42.1 Wed 17:00 ZEU/0260

Mesopores filled with (poly)ionic liquids: phase transitions under confinement, and structure seen by SAXS and SANS — •Julian Oberdisse and Anne-Caroline Genix — Laboratoire Charles Coulomb, U Montpellier France

Understanding the molecular structure of mesoporous solid ionic systems is crucial for optimizing macroscopic properties, in particular ionic transport for energy applications, as well as mechanical flexibility. These systems can be synthesized efficiently under "one-pot" conditions, which rely on mesopore formation through microphase separation of templating ionic liquids.

In the present study, the phase transitions of the embedded ionic liquid have been studied by wide-angle scattering, QENS, DSC, and BDS, as a function of confinement. Then, poly(ionic liquid)s have been added in order to incorporate both connectivity and modify mechanical strength. We report on the structural analysis of ionic liquid and poly(ionic liquid) embedded in ionosilica matrices, employing a combination of small-angle scattering of neutrons and X-rays, isotopic substitution, and physico-chemical solvent-based extraction methods. Data analysis is based on molecular modelling with an original, quantitative comparison of the scattering curves under different contrasts. In agreement with NMR, it is shown that these mesoporous systems have an unexpected molecular structure, with the ionic liquid counterions penetrating the ionosilica matrix surrounding the mesopores. The poly(ionic liquid) forms patches decorating the pore walls, with tunable conformation sensitive to solvent conditions.

CPP 42.2 Wed 17:30 ZEU/0260

Plasmonic core-shell microgels: The role of the core size — •Déborah Feller[1,2], Julian Oberdisse[3], Sylvain Prévost[4], and Matthias Karg[1] — [1]Physical Chemistry of Functional Polymers, Martin Luther University Halle-Wittenberg, Halle (Saale), Germany — [2]Physical Chemistry: Colloids and Nanooptics, Heinrich Heine University Düsseldorf, Düsseldorf, Germany — [3]Laboratoire Charles Coulomb (L2C), Université de Montpellier, CNRS, Montpellier, France — [4]Large Scale Structures, Institut Laue-Langevin, Grenoble, France

Gold-poly-N-isopropylacrylamide (Au PNIPAM) core-shell microgels are interesting due to the localized surface plasmon resonance (LSPR) of the cores. The LSPR position strongly depends on the core size. Compared to other core-shell microgels, Au cores can be precisely overgrown in the shell in situ. Although cores grow in size, the overall hydrodynamic diameter of the microgels does not change. It is not known how the structure of the shell changes during the overgrowth.

Here, we are analyzing Au-PNIPAM microgels with two crosslinker densities. The cores are overgrown from 14 nm in diameter to nearly 100 nm. We perform small-angle X-ray and neutron scattering (SAXS/SANS) to study the respective form factors. SAXS provides information about the cores and SANS about the shell. We also investigate temperature-dependent changes in the microgel by SANS. Additionally, extinction spectra are recorded to study the optical properties. We perform simulations of the different microgels to get information on the internal structure of the shell and the polymer distribution.

CPP 42.3 Wed 17:45 ZEU/0260

Consequences of the near-field effect in highly filled magnetoactive elastomers — •Dirk Romeis and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden

In many theoretical models for magneto-active elastomers (MAEs) the interactions among magnetic/magnetizable particles are approximated via dipole models. In highly filled samples, as well as in structured MAEs, the particles are often very close to each other. In such situation the dipole approximation largely underestimates the interactions among magnetizable particles. Yet, for only 2 spherical particles the analytic solution is quite complex, resulting in a slowly converging series expansion. When considering many particle systems only computationally elaborate methods like a finite element approach can provide numerical solutions. Based on a compact fitting function for the 2-body problem, we suggest an accurate approximation for many-body systems including the near-field effect beyond dipole interactions. Considering these corrections due to the near-field effect in comparison to the dipole approximation, we further investigate the role of cluster formation and dispersion of particles in MAEs when an external magnetic field is applied or switched off.

CPP 42.4 Wed 18:00 ZEU/0260

Magneto-active elastomers with magnetically hard vs soft particles: molecular dynamics simulations — •Júlio P. A. Santos and Sofia Kantorovich — University of Vienna, Faculty of Physics, Kolingasse 14-16, 1090 Vienna, Austria

Magneto-active elastomers (MAEs) [1-2], or magnetorheological elastomers (MREs), are composite materials whose properties - such as stiffness, surface roughness (wettability), and shape - can be controlled by low-energy magnetic fields, making them ideal for soft robotics. MAEs consist of an elastic matrix embedded with magnetic micro- or nanoparticles, magnetically either hard (MH) or soft (MS). For high concentrations of MH particles, one can use a complex arrangement of springs that randomly bond nearby MH particles [3]. However, this model oversimplifies particle behavior (as permanent point dipoles) - critical for modeling physically relevant MAEs.

We address these issues in ESPResSo [4], employing molecular dynamics to study the impact of MS particles on the surface relief of a MAE layer and to provide a critical comparison between MH- and MS-based MAEs. At zero field, MS particles do not interact magnetically, whereas MH particles form long chains within the layer. Increasing the field slowly promotes dipolar interactions between the MS particles and rapidly promotes Zeeman interactions with the applied field, leading to chains that preferentially align parallel to it. In contrast, MH chains must break before reorienting in the direction of the magnetic field, due to the greater importance of dipolar interactions relative to Zeeman, requiring larger applied fields for signficant surface structural changes.

CPP 42.5 Wed 18:15 ZEU/0260

Microstructure analysis of intermediate states in the structure formation process of magnetorheological elastomers — •Nils Magin and Stefan Odenbach — TU Dresden

A composite of magnetic particles and an elastic polymer matrix is referred to as a magnetorheological elastomer. The size and concentration of magnetic particles, as well as the elasticity of the matrix, are the determining factors in the magnetorheological (MR) effect of such materials. Materials exhibiting significant MR properties are commonly referred to as MR elastomers. The application of an external homogeneous magnetic field during the polymerisation process enables the structuring of particles in the initially liquid polymer matrix, resulting in the fabrication of an anisotropic (or structured) material. In order to facilitate a more profound comprehension of the structural formation, the application of the magnetic field is initiated at discrete phases of the polymerisation process. This process gives rise to intermediate states in the structuring that can be observed. The microstructure is examined using computer X-ray tomography and image processing. Furthermore, the influence of the magnetic field, particle concentration, and sample height on the microstructure is discussed. We acknowledge support by the German Research Foundation DFG through Research Unit FOR 5599 on structured magnetic elastomers.

CPP 42.6 Wed 18:30 ZEU/0260

Approximate doubling of the magnitude of maximized magnetorheological effects — Lukas Fischer[1,2] and •Andreas M. Menzel[1] — [1]Otto von Guericke University Magdeburg, Magdeburg, Germany — [2]The University of Osaka, Osaka, Japan

In its static limit, the magnetorheological effect of magnetic elastomers implies changes of elastic moduli by external magnetic fields. Induced magnetic interactions between magnetizable inclusions in a soft, elastic, polymeric matrix affect the overall mechanical stiffness.

First, we optimized the spatial arrangement of the magnetizable inclusions to achieve the strongest change in overall elastic moduli, either for maximized overall stiffening or softening [1]. We focused on both, Young and shear moduli.

Second, in combination, we simultaneously optimized the structural organization to achieve maximized stiffening when an external magnetic field is applied in one direction, but maximized softening when the field is applied along a perpendicular direction [2]. In our case, switching between these two field directions can approximately double the magnitude in overall change of elastic moduli.

Once experimental realizations of prescribed structuring become possible, our strategy provides a direct route to further extend the potential of the materials.

We acknowledge support by the German Research Foundation DFG through Research Unit FOR 5599 on structured magnetic elastomers.

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

[2] L. Fischer, A. M. Menzel, arXiv:2507.22777 (2025).

CPP 43: Biomaterials and Biopolymers (joint session BP/CPP)

Time: Thursday 9:30–12:45 Location: BAR/SCHÖ

CPP 43.1 Thu 9:30 BAR/SCHÖ

Characterization and Application of Honey-PVA Electrospun Scaffolds in Tissue Engineering — •Catalina Navarrete-Vera[1], Karen Yáñez[2], Cristian Acevedo[2], and Tomas Corrales[1,2] — [1]Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile — [2]Centro de Biotecnología Daniel Alkalay Lowitt, Universidad Técnica Federico Santa María, Chile

Tissue engineering seeks to develop functional biomaterials that integrate seamlessly with biological systems. Electrospinning with static collectors enables the production of nanostructured scaffolds suitable for cell regeneration (10.1021/acsomega.3c06436). Incorporating natural components, such as honey, valued for its regenerative, anti-inflammatory, and antimicrobial properties, offers a route to bioactive wound-dressing alternatives (10.1016/j.carbpol.2019.05.004).

In this study, Manuka and Ulmo honeys were each combined with PVA to generate nanofibers and scaffolds via electrospinning. AFM force spectroscopy was used to assess individual fiber mechanics, and SEM and cell-culture assays were employed to evaluate morphology and biocompatibility. Both formulations produced fibers of similar diameter (100-300 nm) and nanomechanical stiffness (˜200 MPa), while honey-containing scaffolds improved cell growth over controls. These results indicate that Ulmo honey is a promising alternative to Manuka honey for tissue-engineering applications.

CPP 43.2 Thu 9:45 BAR/SCHÖ

Additive Manufacturing in Wound Care Innovation from Sugarcane Bagasse — •Ahmed El-Hussein Elnewishy[1], Muhammad Mounir[1], Mona Tarek[1], and Ita Junkar[2] — [1]Biotechnology Program, Faculty of Science, Galala University — [2]Department of Surface Engineering, Jožef Stephan Institute, Ljubljana, Slovenia

Three-dimensional (3D) printing technology is capable of creating highly complex, customizable objects, offering unique advantages for various biomedical applications through methods such as inkjet-based, extrusion-based, and light-assisted techniques. This study focuses on using direct ink writing for additive manufacturing to print antibacterial wound dressings, addressing a critical gap in the current wound care market. The management of chronic and acute wounds presents significant challenges facing human health and overall wellness. Current wound dressing fails to meet patients needs in terms of high adhesion, poor gas exchange, low moisture retention, and the use of systemic and synthetic antibiotics. Additionally, the presence of unused agricultural waste and weak waste management increase greenhouse gas emissions, thus contributing to global warming. To address these issues, we utilized agricultural waste, specifically sugarcane bagasse, to create biopolymer 3D printing ink for wound dressings. We extracted cellulose from sugarcane bagasse and antibacterial bioactive compounds from plant extracts. The synthesized ink was then printed and post treated to enhance mechanical properties. We evaluated the cytotoxicity, antibacterial activity, and morphological structure of the patches using scanning electron microscopy.

CPP 43.3 Thu 10:00 BAR/SCHÖ

FCS-Based RNA Payload Quantification and FLIM Analysis of pH-Dependent Lipid Phase Transitions in Lipid Nanoparticless — •Bernhard Kirchmair[1], Judith Müller[1], Thomas Kellerer[2], Ekaterina Kostyurina[1], and Joachim Rädler[1] — [1]Ludwig-Maximilians-Universität München, Germany — [2]Max Planck-Institut für Biochemie, Martinsried, Germany

Lipid nanoparticles (LNPs) emerged as one of the most promising delivery systems for transfecting mammalian cells with synthetic messenger RNA (mRNA). However, LNPs show a substantial heterogeneity both in shape and cargo and the precise mRNA payload and stoichiometric ratios in multi-component nucleic acid delivery remain poorly quantified. In this project we investigate how mRNA payload depends on LNP size and surface composition using fluorescence correlation spectroscopy (FCS) supported by dynamic light scattering, enabling estimation of particle concentration and RNA copies per LNP. Fluorescence cross-correlation spectroscopy further allows measurement of siRNA/mRNA ratios in mixed cargos. To link payload properties to endosomal escape rates and hence delivery efficiency, we probed pH-dependent lipid phase transitions using fluorescence lifetime imaging (FLIM) and fluorescence anisotropy, capturing changes both in bulk lipid phases and in intact LNPs. These measurements build a framework to monitor structural changes relevant to endosomal escape and can be applied to other LNP formulations and cargo types. Quantitative knowledge about content and ratios will ultimately support the delivery of genetic programs for regulated gene expression.

CPP 43.4 Thu 10:15 BAR/SCHÖ

pH-dependent phase transitions in ionizable lipid mesophases — •Ekaterina Kostyurina[1], Susanne Liese[2], Akhil Sudarsan[2], Julian Philipp[1], and Joachim Rädler[1] — [1]Faculty of Physics, Ludwig-Maximilians University, 80539 Munich, Germany — [2]Faculty of Mathematics, Natural Science, and Materials Engineering, Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

Lipid Nanoparticles (LNPs) have proven valuable in modern medicine as a medium for RNA delivery. Nanoparticles containing cationic ionizable lipid (CIL), cholesterol and structural lipids complex with nucleic acids into size-controlled particles that transport nucleic acid molecules across cell membranes via the endocytic uptake pathway. The delivery efficiency of a drug or vaccine is directly related to the efficiency of the endosomal release. Here, we study pH-dependent structural transitions of the CIL core phase which are believed to play an essential role in this process. We use bulk phases of ionizable lipid/cholesterol as a model system of the LNP core which allows us to study the structure of the lipid phases with high precision using X-ray diffraction. We show that the commonly used ionizable lipids overcome the inverted micellar-inverted hexagonal phase transition within the pH range typical for endosomal life cycle, and connect structural properties of the phases with LNP efficacy. Furthermore, we are aiming to understand the thermodynamics of these phase transitions by combining experimental measurements with theoretical modeling. This will help to better understand the structure-activity relation of LNPs and to increase the delivery efficiency in clinically relevant LNP delivery systems.

CPP 43.5 Thu 10:30 BAR/SCHÖ

To gel or not to gel? Assembly phase changes of engineered spidroin proteins induced by temperature and time — •Isabell Tunn[1,2,3], Dmitry Tolmachev[2,4], Adam L. Harmat[2,4], Nea B. Möttönen[1,2], Alberto Scacchi[2,4,5], Maria Sammalkorpi[2,4], and Markus B. Linder[1,4] — [1]Department of Bioproducts and Biosystems, Aalto University, Finland — [2]Academy of Finland Center of Excellence in Life-Inspired Hybrid Materials (LIBER), Aalto University, Finland — [3]Fraunhofer Institute for Applied Polymer Research (IAP), Germany — [4]Department of Chemistry and Materials Science, Aalto University, Finland — [5]Department of Mechanical and Materials Engineering, University of Turku, Finland

Bioinspired silk-like proteins offer exciting possibilities for developing the next generation of advanced materials - from medicine to food packaging. Here, we investigate the temperature- and time-dependent assembly behaviour of engineered silk-like proteins into hydrogels conducting experiments and molecular dynamics simulations.* Phase transitions are controlled by entropic changes in flexible glycine-rich regions and hydrophobic interactions of alanine-rich α-helical regions. High-temperature gelation proceeds through interactions between alanine-rich domains, leading to β-sheet formation while time-induced gelation occurs via protein percolation mainly driven by dimerization of terminal domains. These findings provide guidelines for engineering protein-based materials with tailored assembly properties and gel characteristics, advancing the rational design of biomimetic soft materials. *https://doi.org/10.1016/j.ijbiomac.2025.147712

CPP 43.6 Thu 10:45 BAR/SCHÖ

Power-Law Analysis of Force Relaxation and Creep Compliance in Nanoindentation of Glassy Gelatin in Humid Air — Paul Zech, Martin Dehnert, Mario Zerson, and •Robert Magerle — Fakultät für Naturwissenschaften, TU Chemnitz

Gelatin-based materials are widely used in food technology, drug delivery systems, and tissue engineering. Water acts as a plasticizer, softening gelatin and reducing its glass transition temperature. Using AFM-based nanoindentation experiments, we examined the mechanical response of a gelatin film to nanoindentations under constant strain (force relaxation) or constant stress (creep compliance) at a wide range of tip approach velocities and relative humidity levels. Scaling analysis using a fractional rheology model reveals that force relaxation and creep compliance exhibit universal power-law behavior. Temporal evolution depends only on the tip indentation time, which defines the externally imposed timescale of the process, and the power-law exponent α, which characterizes the degree of viscoelasticity. At relative humidity $> 85\%$, the α values differ between the force relaxation and creep compliance data. This indicates differences in the underlying molecular processes.

15 min. break

Invited Talk CPP 43.7 Thu 11:15 BAR/SCHÖ

Directed evolution of material-producing bacteria — •André Studart — Complex Materials, Department of Materials, ETH Zürich

Engineers often use high temperatures, pressures and polluting chemicals to make synthetic materials. By contrast, biology produces remarkable materials like wood and bone using widely available chemicals in water and at ambient temperature. The ability of organisms to create materials under mild conditions relies on the intricate biological machinery of living cells. Notably, natural selection processes have evolved such machinery for hundreds of millions of years to fulfill the demands of biological environments. Can we harness the machinery and evolutionary processes of biology to create materials more sustainably while still meeting engineering needs ? To explore this question, we utilized a microfluidic platform to evolve material-forming microorganisms towards cell mutants that meet the high productivity needed in industrial processes. Using cellulose-producing bacteria as an example, we show that this directed evolution approach enabled the isolation of a bacterial mutant that produces up to 70% more cellulose than its native counterpart. The overproducing bacterial strain offers an attractive alternative to wood to meet the growing demand for cellulose in the textile, medical and packaging industries. Beyond cellulose, the proposed technology offers a compelling approach to isolate bacteria for the bio-fabrication of other sustainable materials, such as silk, polyesters and clay-based bricks.

CPP 43.8 Thu 11:45 BAR/SCHÖ

Controlling Axonal Outgrowth of Organoids by 3D Nanoprinted Scaffolds — •Tobias Müller[1], Malte Siegmund[1], Emma Wollesen[1], Kim Krieg[2], Ole Pless[2], Jan Hahn[3], Robert Zierold[1], and Robert Blick[1] — [1]Center for Hybrid Nanostructures, University of Hamburg, 22761 Germany — [2]Fraunhofer ITMP, Discovery Research Screening Port, 22525 Germany — [3]Section Facility Mass Spectrometry and Proteomics, University Medical Center Hamburg-Eppendorf, 20246 Germany

Cortical organoids are promising models for neurodegenerative disease research, yet their integration into defined neural networks remains challenging. We use two-photon polymerization (2PP) to fabricate three-dimensional scaffolds that direct axonal outgrowth and support organoid integration into engineered circuits.

Scaling structures from single neurons to millimeter-scale organoids introduces adhesion and imaging challenges. We address this by combining tailored scaffold geometries with a polydimethylsiloxane (PDMS)-based anchoring strategy, critical-point drying and quantitative analysis of electron microscopy images. Walls, stairs and microwires enhance organoid-scaffold interactions, promoting axonal outgrowth along intended paths and reducing extension into non-target regions.

These results demonstrate that 2PP-fabricated microarchitectures can guide axon growth and stabilize organoid-substrate contact, enabling more controlled organoid-based neuronal networks and advancing brain-on-a-chip approaches.

CPP 43.9 Thu 12:00 BAR/SCHÖ

Stimulus-induced biomechanical perturbations via smart hydrogel microstructures — •Katja Zieske — Max Planck Institute for the Science of Light, Erlangen, Germany

Cells reside within complex three-dimensional extracellular matrices, where mechanical interactions play essential roles in tissue development, and disease progression. To mimic these interactions, we developed a lab-on-a-chip platform that applies spatially and temporally controlled mechanical perturbations using intelligent hydrogel microstructures.

First, we optimized material composition and photopolymerization parameters and demonstrated reliable, stimulus-dependent expansion and contraction of the hydrogel microstructures within microfluidic chambers. Using these microstructures, we then applied compressive forces to Matrigel and collagen networks. Finally, we applied mechanical perturbations to cellular systems.

By mimicking cellular pushing forces with hydrogel microstructures, this lab-on-a-chip system provides a versatile tool for studying mechanical remodeling of biopolymers and cellular systems.

CPP 43.10 Thu 12:15 BAR/SCHÖ

Functionally Connecting High- and Low-Density Neuronal Networks Using 3D-Nanoprinted Structures — •Emma Wollesen, Malte Siegmund, Tobias Müller, Josephine Hoppe, Robert Zierold, and Robert Blick — Center for Hybrid Nanostructures, University of Hamburg, 22761 Hamburg, Germany

Tracing the propagation of interneural communication from high- to low-density networks is essential for exploiting information processing at the single-cell level. Given the multitude of synaptic connections, high-density networks of hiPSC-derived neurons may generate bursts of action potentials, a key communication mode that can be analyzed at the single-cell level in receiving low-density networks. Here, we move toward such a cultivation platform by evaluating 3D nanoprinted (3DN) structures fabricated by two-photon polymerization for their efficiency in facilitating connected high- and low-density networks. We demonstrate the prerequisite formation of hiPSC-derived low-density neuronal networks in tower-shaped 3DN structures. For augmentation with high-density networks, a stomach-shaped structure and connecting elements were fabricated. A minimum structure height of 30 micrometers proved critical for clear network demarcation. For future region-specific chemical stimulation, millimeter-scale structures for media reservoir separation were conceptualized, and fabrication feasibility was confirmed, requiring a 10 micrometer overlap and a suitable shear angle at structure interfaces. These results extend established 3DN platforms for low-density networks and support the integration of neural networks into Brain-on-a-Chip applications.

CPP 43.11 Thu 12:30 BAR/SCHÖ

Multiplex sensing of respiratory viruses using surface plasmon resonance spectroscopy — •Ghazaleh Eshaghi[1], David Kaiser[1], Hamid Reza Rasouli[1], Dominik Gary[2], Tobias Fischer[2], Katrin Frankenfeld[2], Abhishek Sharma[3], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Forschungszentrum für Medizintechnik und Biotechnologie (fzmb) GmbH, 99947 Bad Langensalza, Germany — [3]BioNavis Ltd., Hermiankatu 6-8H, 33720 Tampere, Finland

We present label-free and real-time biosensing of three major respiratory viruses using the Multi-Parametric Surface Plasmon Resonance (MP-SPR) technique. In this approach, MP-SPR SPR Au sensors are functionalized with ultrathin (~1 nm) azide-terminated carbon nanomembranes (N3-CNMs), enabling covalent attachment of virus-specific antibodies and thereby providing selective immobilization of target antigens on the sensor surface. We demonstrate specific detection of SARS-CoV-2, Influenza A, and Respiratory Syncytial Virus (RSV) antigens with negligible cross-reactivity and high reproducibility in both PBS-P buffer (physiological pH) and clinically relevant nasopharyngeal swab matrices. For SARS-CoV-2, Influenza A, and RSV antigens, we determine dissociation constants (KD) of 7.0 * 0.5 nM, 86 * 4 pM, and 3.0 * 0.2 pM, respectively, with corresponding limits of detection (LOD) of ~65 pM, ~80 pM, and ~2 pM.

CPP 44: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics V

Time: Thursday 9:30–11:15 Location: ZEU/LICH

Invited Talk CPP 44.1 Thu 9:30 ZEU/LICH

Shedding light on wide bandgap perovskites — •Michael Saliba — Institute for Photovoltaics (ipv), University of Stuttgart, Germany

Low bandgap perovskite solar cells are approaching the Shockley-Queisser limit for single-junction solar cells. Less progress, however, was made for wider bandgap perovskites, which are of interest, e.g., for multijunction photovoltaics. These wide bandgap perovskites are often comprised of fully inorganic components, which are hard to dissolve in conventional solvent systems and require more sophisticated synthesis as well as crystallisation techniques. In this talk, I will discuss strategies to address these challenges by providing a library of hitherto unexplored wider bandgap perovskites using combinatorics.

Unfortunately, the newly formulated liquid precursors often exhibit complex crystallization behaviour struggling to expel the typically used DMSO solvent. To delay the crystallization time, two strategies are proposed to remove the strongly complexating DMSO molecules through a) modified processing of the liquid thin-film and b) a coordination solvent with a high donicity and a low vapor-pressure leading to a marked improvement in the overall film quality. Lastly, interface manipulation, especially on top of the formed perovskite, is becoming a central topic to advance further. Light annealing is introduced to modify the perovskite surface resulting in a reduced surface recombination.

CPP 44.2 Thu 10:00 ZEU/LICH

Perovskite Solar Cells under Orbit-Like Thermal Cycling — •Simon Alexander Wegener[1], Christoph Gernot Lindenmeir[1], Thomas Baier[1], Xiaojing Ci[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, Trieste, Italy

Perovskite solar cells offer strong potential for space power systems due to their high visible-light absorbance, thin active layers, and efficiencies comparable to silicon. These features provide exceptional power-to-weight ratios, and solution processing reduces manufacturing and launch costs relative to multi-junction gallium arsenide cells. Initial demonstrations have confirmed their operability in space. Key challenges remain, particularly the extreme temperature swings in low Earth orbit. Our work examines these stresses using operando grazing-incidence wide-angle X-ray scattering (GIWAXS) to track structural changes in the perovskite during illumination and temperature cycling. Synchrotron radiation enables the necessary temporal resolution to study the multilayer device stack, which combines materials with differing mechanical and thermal properties. Complementary photoluminescence measurements reveal associated changes in optical and electrical behavior. Across -125°C to +100°C, the perovskite shows changes in crystal phase, anisotropic strain, and optoelectronic response. These findings clarify the coupled mechanical and electronic effects driving performance loss and enable strategies to enhance durability of perovskite solar cells for space applications.

CPP 44.3 Thu 10:15 ZEU/LICH

Depth Resolved Structural Analysis on CsPbI3 Nanocrystal Nucleation Seed Induced Pervskite Thin Films — •Altantulga Buyan-Arivjikh[1], Lukas Wolz[1], Ajeet Kumar[2], Yanan An[1], Christopher Everett[1], Guangjiu Pan[1], Jinsheng Zhang[1], Zhuijun Xu[1], Matthias Schwartzkopf[3], Stephan V. Roth[4], Jürgen Hauer[1], Johanna Eichhorn[1], and Peter

Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, 85748 Garching, Germany — [2]Department of Chemical Physics, Lund University, 22100 Lund, Sweden — [3]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [4]Department of Fibre and Polymer Technology KTH, SE-10044 Stockholm, Sweden

Lead-halide perovskites have attracted significant attention due to their favorable optoelectronic properties, simple processing, and the availability of precursor materials. Their performance is strongly governed by the crystallinity and morphology of the typically polycrystalline thin films. Among strategies to optimize these features, nanocrystal seeding has emerged as a promising route. Here, we show improved crystallographic orientation and reduced defect density in printed FAPbI3 thin films through the introduction of CsPbI3 nanocrystal nucleation seeds. Incidence-angle-varied GIWAXS enabled depth-resolved structural analysis, revealing seed incorporation and corresponding modifications of the energy landscape through the film thickness.

CPP 44.4 Thu 10:30 ZEU/LICH

***In-Situ* KPFM Growth Studies of Pentacene as a Model Hole Transport Material on 2D/3D Heterostructured Cs$_2$AgBiBr$_6$ for Perovskite Solar Cells** — •Tim P. Schneider and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Forming low-dimensional perovskite interlayers in perovskite solar cells by applying ammonium salt solutions is a well-known method to improve devices. This has already been approved for the Cs$_2$AgBiBr$_6$ double perovskite in solar cell geometry by a 2D-modification with BABr or PEABr salts achieving respective low-dimensional phases at the interface. Using pentacene as a model hole conductor, its film growth and contact formation to the different double perovskite phases was investigated via *in-situ* growth studies using Kelvin Probe force microscopy (KPFM). Measuring the morphology and work function at intermittent steps during film deposition allowed to observe their evolution depending on the average pentacene film thickness. Image processing of the resulting KPFM images facilitated to assign different morphological features (from substrate or pentacene) present in the height images to different contributions to the work function and, especially, clearly identified the pentacene grains within other similar morphological features. A much more homogenous growth of pentacene on 2D/3D heterostructured Cs$_2$AgBiBr$_6$ was observed, forming evenly shaped grains or dendritic islands. This was further accompanied by a more confined work function, speaking for an enhanced contact alignment between the double perovskite and pentacene.

CPP 44.5 Thu 10:45 ZEU/LICH

Gas quenching under ambient condition for efficient and stable perovskite solar cells with surface passivation — •Zhaonan Jin[1], Xiongzhuo Jiang[1], Zerui Li[1], Xiaojing Ci[1], Guangjiu Pan[1], Lixing Li[1], Jinsheng Zhang[1], Xinyu Jiang[2], Sarathlal Koyiloth Vayalil[2,3], Kun Sun[4], Stephan V.Roth[2,5], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]DESY, Hamburg — [3]UPES, India — [4]HZB, Berlin — [5]Department of Fibre and Polymer Technology, KTH, Stockholm, Sweden

Wide-bandgap perovskite solar cells play a key role in tandem solar cells, which aim to overcome the Shockley-Queisser limit for single-junction solar cells. In this work, we develop and optimize a gas quenching method under ambient conditions for the fabrication of wide-bandgap (1.77 eV) perovskite films. To improve the performance of PSCs, three different organic spacer cations, including aromatic amino molecules (PEAI), aliphatic amino with long alkyl chain molecules (OAI), and short alkyl chain molecules (BAI), are applied and investigated as surface passivation materials. As a result, the 2D perovskite layers form on top of 3D perovskite films. The n-i-p devices with PEAI passivation exhibit a champion PCE of 16.26% along with a high Voc of 1.21 V, exceeding the control device (PCE = 13.42%, Voc = 1.15 V), and maintaining 88% of its initial PCE after 120 minutes of continuous illumination. This work offers a guide for the fabrication of wide-bandgap PSCs under ambient conditions and the choice of organic spacer cations for passivation.

CPP 44.6 Thu 11:00 ZEU/LICH

Solvated PbI2 Clusters Preceding the Crystalization of Lead Halide Perovsites - UV/VIS In Situ Study — •Maximilian Spies[1], Leonard Krapf[1], Fabian Eller[2], Eva M. Herzig[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth — [2]Dynamics and Structure Formation, University of Bayreuth

The solution-based fabrication of reproducible, high-quality lead iodide perovskite films demands a detailed understanding of the crystallization dynamics. This dynamic is primarily determined by the precursor solution chemistry and processing conditions. We conducted a systematic in-situ study to elucidate the formation mechanism of perovskite films and the role of additives in the pre-crystallization phase. Using UV absorption spectroscopy during spin coating allows us to track the evolution of iodoplumbate complexes and a solvated pre-crystalline phase (PDS) present in the precursor solution. This PDS phase is proportional to the precursor concentration, even during spin coating. Notably, using different precursor solvents changes the PDS phase evolution substantially. However, when introducing additives we see no difference in this pre-crystalline evolution, suggesting that additives only affect the perovskite film formation at a later stage

CPP 45: Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates I (joint session CPP/BP)

Biomolecular condensates play a central role in many cellular processes and provide a fascinating example of self-organized, highly dynamic systems. Physical methods, particularly from statistical physics and soft matter, have emerged as valuable tools for understanding and predicting their fundamental properties. Conversely, the complexity and diversity of biological systems open new perspectives and challenges for physical modeling. This focus session will highlight current research at the interface of physics and biology, with an emphasis on theoretical modeling and simulation of the physics of biomolecular condensates.

Organized by Arash Nikoubashman, Tyler Harmon and Lukas Stelzl.

Time: Thursday 9:30–11:15 Location: ZEU/0260

Topical Talk CPP 45.1 Thu 9:30 ZEU/0260

Wetting transitions in biomolecular coacervates — •Susanne Liese[1], Tiemei Lu[2], Evan Spruijt[3], and Christoph Weber[1] — [1]University of Augsburg — [2]University of Oxford — [3]Radboud University

Biomolecular coacervates are liquid-like droplets that can interact with membranes and self-organize into complex structures. Understanding the principles governing their shapes and higher-order assemblies is crucial for controlling compartmentalization in biological and synthetic systems.

We present a theoretical framework describing the shape and organization of biomolecular coacervates interacting with membranes and each other. Large coacervate droplets adopt morphologies determined by the balance of surface tensions, from partial adhesion to full engulfment. Scaled membrane tension and droplet-membrane interactions predict transitions between spherical, lens-shaped, partially wrapped, and endocytosed droplets, with composition-dependent contact angles linking molecular properties to macroscopic shapes.

For multiphase coacervates, we model the impact of interfacial species on droplet organization. Enrichment of an interfacial component at phase boundaries drives partial wetting between droplets, promoting the formation of dimers and extended chains. Numerical simulations show that surface tension minimizes the contact area, straightening droplet arrangements and generating polymer-like behavior with bending stiffness and segment-length constraints.

CPP 45.2 Thu 10:00 ZEU/0260

Elastic regulation of biomolecular condensates — •Oliver Paulin and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

In recent years, biomolecular condensates have emerged as a vital component of sub-cellular organisation. Here, we discuss the role that elastic interactions can play in regulating condensate size, count, and mechanical properties. First, we focus on the impact of ‘external’ elasticity that arises from a confining mesh such as the cytoskeleton. We find that the additional energetic cost of network deformations induced by condensate growth limits condensate size, and can even suppress condensate formation entirely. Additionally, when condensate size is comparable to characteristic heterogeneities of the network, non-local interactions may arrest thermodynamic coarsening and drive the formation of stable patterned states with an energetically selected length scale. Second, we study how ‘internal’ elasticity, resulting from the intrinsic viscoelasticity of condensate material, can inhibit condensate growth, but also impart condensates with mechanical strength. For the case in which condensate growth is driven by active incorporation of new material, we demonstrate how a delicate balance of material properties provides condensates with solid-like mechanical strength, without compromising their liquid-like ability to form and grow rapidly. For both examples, we construct dynamic continuum models that couple phase separation with elastic deformation, analysing the key parameters that control condensate form, and identifying how cells can use elasticity to fine-tune condensate behaviour to fulfil a specific function.

CPP 45.3 Thu 10:15 ZEU/0260

Phase Separation of a Nucleator in a Self Straining Active Filament Network — •Jakob Schindelwig[1], Quentin Bodini-Lefranc[1,2], and Sebastian Fürthauer[1] — [1]Institute of Applied Physics, TU Wien, Lehargasse 6, 1060 Vienna, Austria — [2]Ecole polytechnique, Institut Polytechnique de Paris, Route de Saclay, 91120 Palaiseau, France

Many membraneless compartments of cells, such as stress-granules, form via liquid-liquid phase separation. In cells many compartments of the same type and similar sizes can coexist. Since this is inconsistent with equilibrium phase separation physics, we ask if active mechanics could explain this observation. We develop a model coupling dynamics of the droplet material to an active self-straining filament network. This model shows (i) arrested coarsening , (ii) oscillations, (iii) scale selection. We establish that our model is physiologically plausible by comparing to recent work on a phase separating nucleator of actin.

CPP 45.4 Thu 10:30 ZEU/0260

Active Transport as a Mechanism of Microphase Selection in Biomolecular Condensates — •Le Qiao, Peter Gispert, and Friederike Schmid — Institut für Physik, Johannes Gutenberg-Universität Mainz, D55099 Mainz, Germany

Cells control the size and organization of biomolecular condensates formed by liquid-liquid phase separation (LLPS), yet the underlying physical principles remain incompletely understood. We propose a transport-driven mechanism in which undirected motor-mediated motion along cytoskeletal filaments redistributes phase-separating components, generating an effective non-equilibrium long-range repulsion that arrests coarsening. This is explored using a minimal reaction-diffusion-transport model that captures the interplay between binding-release kinetics, diffusion, and active transport. A linear stability analysis and three-dimensional simulations reveal a transition from macroscopic to microphase separation at remarkably low binding/release fractions, corresponding to minute fractions of motor-bound proteins. Tuning motor binding rates b or transport velocities enables sublinear control of condensate dimensions ($L \sim b^{1/4}$) from nanometers to micrometers. This mechanism provides a simple physical route for spatially programmable condensate organization in living cells and active materials.

CPP 45.5 Thu 10:45 ZEU/0260

Positive feedback in chemically active droplets — •Xi Chen[1], Jens-Uwe Sommer[1,2], and Tyler Harmon[1] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]Dresden University of Technology

Biomolecular condensates are dynamic compartments that can be maintained far from equilibrium by active chemical reactions. Active condensates can be driven by phase-dependent reaction fluxes, for example via localized enzymatic activity, and thereby exhibit emergent behaviors that cannot be realized in equilibrium condensates. We analyzed condensates with positive feedback between phase separation and reactions: droplets enhance reactions, and the resulting products stabilize the droplets. We show that this feedback produces pronounced hysteresis, making droplets resilient to cellular fluctuations. We show the hysteresis persists across a broad range of reaction schemes and parameter choices, indicating that it is a robust feature of droplets with positive feedback. Condensates that form to satisfy transient cellular needs may benefit from such hysteresis, because it ensures that they persist long enough to carry out their functions despite fluctuating conditions.

CPP 45.6 Thu 11:00 ZEU/0260

Chemically driven simulations of enzymatic phosphorylation in protein condensates — •Emanuele Zippo[1], Dorothee Dormann[1,2], Thomas Speck[3], and Lukas Stelzl[1,2] — [1]Johannes Gutenberg University Mainz, Mainz, Germany — [2]Institute of Molecular Biology (IMB), Mainz, Germany — [3]University of Stuttgart, Stuttgart, Germany

The condensation and aggregation of intrinsically disordered proteins (IDPs) in cells are governed by enzyme-driven, non-equilibrium processes. Kinases such as Casein kinase 1 delta (CK1d) phosphorylate proteins using ATP as chemical fuel, tuning intermolecular interactions and modulating condensate assembly. The neurodegeneration-linked protein TDP-43 undergoes CK1d-mediated hyperphosphorylation, proposed as a cytoprotective mechanism through condensate dissolution, yet the mechanisms underlying kinase-condensate interactions remain unclear. Using coarse-grained molecular dynamics simulations, we investigate how CK1d phosphorylates TDP-43 and how this reaction drives the structural reorganization and dissolution of its condensates. To ensure thermodynamic consistency in such fuel-driven simulations, we employ an automatic, generally applicable Markov state modeling framework. Post-translational modifications (PTMs), such as phosphorylation, can actively regulate condensate stability and suppress Ostwald ripening, offering a mechanism to control mesoscale structure in soft materials. Understanding such reaction-structure coupling in non-equilibrium environments is key to explaining cellular self-organization and designing biomimetic systems.

CPP 46: Poster II

Focus Session: Water - from Atmosphere to Space (with DY); French-German Session: Membranes and Porous Materials; Gels, Polymer Networks and Elastomers; Biopolymers, Biomaterials and Bioinspired Functional Materials (with BP); Complex Fluids and Colloids, Micelles and Vesicles (with DY); Charged Soft Matter, Polyelectrolytes and Ionic Liquids; Responsive and Adaptive Systems; Nanomaterials, Composites and Hybrids; Crystallization; Molecular and Polymer Dynamics, Friction and Rheology; Simulation Methods and Modeling of Soft Matter; Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods

Time: Thursday 9:30–11:30 Location: P5

CPP 46.1 Thu 9:30 P5

Pressure-induced amorphization of aqueous PEG solutions — •Leah Dorothea Schwerdtfeger[1,2], Isabell Zick[1,2], and Katrin Amann-Winkel[1,2] — [1]Institut für Physik, Johannes Gutenberg Universität, Mainz — [2]Max-Planck-Institut für Polymerforschung, Mainz

Water is a fundamental substance whose behavior under supercooled temperatures shows many anomalous properties. Among the many curiosities, water can even form different amorphous states. These amorphous states are hypothesized to be directly related to two different liquid states of water, namely high- and low-density liquid. Understanding the pressure-induced amorphization of aqueous solutions can reveal how solutes alter water's phase diagram and give further insight to the predicted liquid-liquid transition.

While the impact of small molecules is known from previous studies, the role of larger polymers remains unexplored. Here, we discuss experiments on aqueous polyethylene glycol (PEG) solutions with different molar weights, studying their effect on the pressure-induced phase transitions. Our dilatometric measurements show how solutes broaden the transition from hexagonal ice to high-density amorphous ice (HDA), depending on the molar fraction. We also investigate the polyamorphic transition between low- and high-density amorphous ice (LDA-HDA), which for pure water is known to exhibit a strong temperature-dependence. The samples are further characterized by X-Ray diffraction (XRD).

CPP 46.2 Thu 9:30 P5

Phase transition in water-glycerol solutions — •Klara Holl[1,2], Louisa Kraft[1,2], and Katrin Amann-Winkel[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität, Mainz — [2]Max-Planck-Institut für Polymerforschung, Mainz

Water is omnipresent in our daily lives with many anomalous properties and a unique phase diagram. Studies of supercooled water provides insight into the hypothesis of the coexistence of two liquid states of water and a liquid-liquid transition. This proposes two different types of supercooled liquid water in a high-density and low-density liquid state, that are separated by a first order phase transition at low temperatures and elevated pressure. But how does this hypothesis impact on aqueous solutions?

Water-glycerol mixtures are often used in pharmaceuticals and act as cryoprotectants, common in biomedicine as well as automotive antifreeze. While pure water crystallizes easily, the glass-forming agent glycerol can serve as soft confinement for water. Changing the concentration of the two components alters the liquid's physical and thermodynamic properties, including depression of the crystallisation temperature.

We investigate different water-glycerol solutions at low-temperatures and high-pressure conditions using a diamond anvil cell. This allows in situ optical observation of crystallisation and glass transition. Structural changes are studied by X-ray diffraction and differential scanning calorimetry.

CPP 46.3 Thu 9:30 P5

Photooxidation of vanillic acid at the air-water interface — •Manuel Hofmann[1,2] and Ellen H.G. Backus[1,2] — [1]Institute of Physical Chemistry, Faculty of Chemistry, University of Vienna, Währinger Str. 42, 1090 Vienna, Austria — [2]University of Vienna, Vienna Doctoral School in Chemistry (DoSChem), Währinger Str. 42, 1090 Vienna, Austria

Phenolic compounds like vanillic acid, emitted from biomass burning, can form secondary organic aerosols (SOA) through aqueous phase reactions. Photooxidation of vanillic acid is a potential source of Humic-Like Substances (HULIS), that influence atmospheric chemistry through light absorption.[1]

The air-water interface provides a distinct chemical environment where structural behavior and reactions may differ from those in bulk. To specifically probe this interface, sum-frequency generation (SFG) spectroscopy and surface tension measurements are employed, offering complementary insights into molecular behavior.[2]

This study examines vanillic acid at the air-water interface across different pH values, before and after UV/H2O2-induced photooxidation. Control experiments with vanillic acid alone separate direct photolysis from radical mediated processes. Preliminary SFG spectra reveal pH-dependent vibrational signatures of adsorbed species and significant changes upon photoreaction. The goal is to identify reaction products, structural changes, and how pH affects vanillic acid photoreactivity.

[1]S. Tang et al., ACS Earth Space Chem., 4 (2020) 862-872.[2]C.-M. Saak et al., J. Phys. Chem. Lett., 15 (2024) 4546-4559.

CPP 46.4 Thu 9:30 P5

Biophysical Interaction of Steroid Hormones with Model Lipid Membranes — •Rabia Rabia[1,2,3], Prashant Hitaishi[1,2], Bridget Murphy[1,2], and Julia Herzen[3] — [1]Institute of Experimental and Applied Physics, Kiel University, Leibnizstraße 19, Kiel, 24118, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, Hamburg, 22607, Germany — [3]Technische Universität München

Menopause is characterized by declining 17βestradiol (E2), increased adiposity, reduced insulin sensitivity, and higher type 2 diabetes risk. Vasomotor symptoms, such as hot flushes and night sweats, significantly impair quality of life, and transdermal E2 provides effective relief at lower doses than oral therapy, with potentially fewer systemic risks. Despite its clinical benefits, the molecular mechanisms of E2 remain incompletely understood. While steroid hormones classically act via intracellular receptors to regulate gene transcription, they also interact directly with lipid membranes, influencing packing and elasticity. We studied βestradiol, progesterone, 17αethynylestradiol, and cholesterol in DPPC and POPC monolayers at the air water interface using Langmuir isotherms and surface elasticity measurements. E2 was found to expand molecular area and reduce packing density, increasing membrane elasticity. Planned X-ray measurements will further clarify how steroid-induced reorganization of lipid interfaces modulates downstream cellular signaling.

CPP 46.5 Thu 9:30 P5

The structure and orientation of ice under confinement in Periodic Mesoporous Organosilicas (PMOs) — Niels C. Giesselmann[1], Philip Lenz[2,3], Sophia-Marie Meinert[2], Robert P.C. Bauer[1,4], Nele N. Striker[1], Michael Fröba[2,3], and •Felix Lehmkühler[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Institute for Inorganic Chemistry, University of Hamburg,Germany — [3]The Hamburg Center for Ultrafast Imaging, Hamburg, Germany — [4]Freiberg Center for Water Research, TU Bergakademie Freiberg, Germany

We studied water in periodic mesoporous organosilicas (PMOs) with pore diameters in the range of 2-5 nm. In these materials, the molecular mobility of water is influenced by the polarity of the organic moiety. We collected and analyzed X-ray scattering data of water and ice under confinement in PMOs with varying degrees of hydrophobicity and pore diameters and at varying temperature. A decrease in the density of the confined water was observed during cooling, which was strongly dependent on the organic moiety, as well as the pore diameter. We furthermore found deviations in the lattice constants of hexagonal ice in these materials compared to bulk water. In most cases, one lattice parameter was more strongly affected. This could be caused by orientational dependencies between the ice crystal and the pore. The orientation between the hexagonal crystallites in relation to the pore axis was therefore investigated using X-ray Cross Correlation Analysis (XCCA), indicating more uniformly oriented crystallites in more hydrophilic pores.

CPP 46.6 Thu 9:30 P5

Impact on snow albedo of soot aggregates inferred from their radiative properties — •Llorenc Cremonesi[1], Luca Teruzzi[1], Valentina Raspagni[2], and Marco Potenza[1] — [1]University of Milan, Milan, Italy — [2]Ca' Foscari University of Venice, Venice, Italy

Despite having a short lifespan in the atmosphere, soot aggregates are abundant and volatile enough to be found in various environments far from their sources. While suspended in the atmosphere, they influence local thermodynamic conditions and interact with water triggering cloud nucleation. These particles are also among the drivers of cryospheric degradation in climate-sensitive areas such as the Arctic and the European Alps.

The effectiveness with which soot aggregates interact with solar radiation is known to be related to their morphology as well as their composition. However, studies of their radiative properties rely on indirect or model-dependent measurements. We use a non-destructive optical technique that enables us to simultaneously measure several optical parameters on a particle-by-particle basis in situ.

Field measurements and laboratory tests show that aggregate particles exhibit exceptional scattering and absorption efficiencies relative to their mass. Directly assessing these properties obviates the need to characterise their exceptional morphological variability. By quantifying these properties, we evaluate the impact of carbon aggregates on snow, particularly in the uppermost layers.

CPP 46.7 Thu 9:30 P5

Study of nuclear magnetization transfer between water and ice phases in nanoporous solids — •Cristina Abril Gutierrez Ortigoza and Rustem Valiullin — Felix Bloch Institute for Solid State Physics, University of Leipzig, Leipzig, Germany

NMR Cryoporometry is a promising tool for the characterization of nanoporous solids. The technique relies on introducing a probe liquid into the nanopores, where a liquid and frozen phase can coexist at low temperatures. Both phases can be easily identified using NMR due to their vastly different transverse relaxation rates. The magnetization transfer mechanism between these is not well understood, especially its dependence on various parameters such as temperature and pore size. In this contribution, the magnetization transfer between water and ice in porous silica is explored, the pore structure of which is composed of well-ordered spherical nanopores connected by micropores. The measurements are performed by using the Goldman-Shen pulse sequence, which initializes the experiments in a state where all the magnetization is contained in the liquid phase. By studying how the system re-equilibrates, parameters such as the diffusion coefficient in the ice phase and the proton volume fraction in each phase are obtained. Furthermore, the non-frozen layer thickness, which refers to the liquid-like layer that forms between the ice core and the pore wall, can be obtained by exploiting the well-defined geometries of the ice and water phases. The studies were performed at different temperatures to assess the dependence of the results on this parameter. The experimental data are also compared to theoretical models.

CPP 46.8 Thu 9:30 P5

Advanced analysis of NMR cryoporometry data — •Crina Rahause, Georgiy Baroncha, and Rustem Valiullin — Felix Bloch Institute for Solid State Physics, Leipzig University, Leipzig, Germany

NMR cryoporometry is a powerful tool for structural characterisation of multi-scale nanoporous materials. It relies on probing the pore size dependent ice-liquid phase transitions of nanoconfined liquid. However, accurate interpretation of the experimental data requires a better description of phase equilibria, as well as a framework that takes into account the network topology and relaxation effects. In this contribution, we perform NMR measurement using water and octamethylcyclotetrasiloxane (OMCTS) as probe liquids inside highly ordered nanoporous alumina membranes with well-defined pore sizes ranging from 25 to 180 nanometres. OMCTS differs from water in terms of relaxation times and the thermodynamic parameters controlling phase transition suppressions; therefore, by comparing the responses of the two liquids in different porous media, we can identify key parameters which are necessary for accurately establishing an advanced cryoporometry methodology, and demonstrating the applicability of this technique to a wide range of materials.

CPP 46.9 Thu 9:30 P5

Comparison of mechanical properties and pore collapse characteristics of hyperuniform disordered anodic aluminium oxide membranes — •Rang Noh[1], Clara Twiehaus[2], Marc Thelen[1], Alexander Sprafke[3], Prerak Dhawan[3], Ralf Wehrspohn[3], Martin Steinhart[2], and Patrick Huber[1,4] — [1]Institute for Materials and X-ray Physics, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Chemistry of New Materials, Osnabrück University, Osnabrück, Germany — [3]Institute of Physics, Martin Luther University of Halle-Wittenberg, Halle (Saale), Germany — [4]Center for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

We investigate how the degree of disorder in hyperuniform Porous Anodic Aluminum Oxide (AAO) membranes influences their mechanical properties and pore-collapse behavior. Elastic moduli of AAO were measured using two different methods; Laser Ultrasonics (LUS) and nanoindentation. The indented points were captured by scanning electron microscopy to observe pore collapse characteristics. The elastic moduli from LUS and nanoindentation agree well; in general, the elastic modulus increases as both porosity and the hyperuniformity index decrease. Even at similar porosity levels, enhanced hyperuniformity results a higher elastic modulus. When the pores are ordered, the pore collapse follows directional grain paths around the indented edge and propagate further in a connected herringbone like pattern. But, in the disordered state, the irregular collapse happens, producing direction-independent crack propagation within the restricted region.

CPP 46.10 Thu 9:30 P5

Microscopic mechanisms of polymer network breakage under mechanical deformation — •Fernando Martín Salamanca[1,2] and Michael Lang[1] — [1]Institute Theory of Polymers, Leibniz-Institut für Polymerforschung Dresden e.V. Kaitzer Strasse, 4 - 01069 (Dresden) — [2]Institute of Polymer Science and Technology, Spanish National Research Council. Juan de la Cierva, 3 - 28006 (Madrid)

The failure of polymer networks arises from a subtle interplay between bond rupture, chain interactions and the underlying topology of the network. In this work, Monte Carlo simulations are used to explore how these factors shape the mechanical response of crosslinked polymers subjected to mechanical stress. The main goal is to evaluate, in a controlled manner, the key elements that modify the mechanical response by computer simulations: the criteria for bond rupture, the mathematical modelling of interactions potentials and force fields, the effect of entanglements and excluded volume. Model networks are evaluated with diverse approaches to quantify the effect of each contribution to elastic modulus. The simulations yield detailed rupture statistics and stress-strain behavior across a broad parameter space, which are compared with predictions from established theoretical descriptions of network elasticity and fracture. Overall, this work provides basic information for understanding network failure and for establishing a first-principles based model for real polymer networks.

CPP 46.11 Thu 9:30 P5

Tuning Foam Kinetics and Structure: The Role of Gas Flowrate in Microgel-Stabilized Foams — •Vera Anna Nina Alina Hesse, Joanne Zimmer, and Regine von Klitzing — Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 8, D-64289 Darmstadt

The stability and microstructure of foams are critical for their performance in various applications. In this work, aqueous foams are generated by sparging gas (nitrogen) through an aqueous dispersion of PNIPAM microgels, which are used as foam-stabilizers. In specific the effect of the gas flowrate during foam production on the foam structure and kinetics is investigated. In this regard, key parameters such as the foam half lifetime, drainage (liquid content), and bubble size evolution are examined. Our findings reveal a clear dependence: In general, lower flowrates produce smaller initial bubbles, which in turn significantly improve the overall foam stability, as their structural skeleton remains intact for longer periods. On the other hand, a stability optimum is detected, with peak stability occurring at a low flowrate; further reduction however ultimately compromising stability. These findings contribute to a deeper understanding of microgel-stabilized aqueous foams and render the potential for optimizing foam generation processes.

CPP 46.12 Thu 9:30 P5

Shape and inner structure of micelles from tetrablock terpolymers in aqueous solution — •Katarina Döbler[1], Feifei

Zheng[1], Pablo A. Alvarez Herrera[1], Joachim Kohlbrecher[3], Anna P. Constantinou[2], Theoni K. Georgiou[2], and Christine M. Papadakis[1] — [1]Technical University of Munich, TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]Imperial College London, U.K — [3]PSI, Villigen, Switzerland

Injectable hydrogels formed by LCST thermoresponsive block terpolymers consisting of thermoresponsive, hydrophilic and hydrophobic blocks are promising materials for tissue engineering by 3D bioprinting. The gel point temperature, gelation mechanism, and physical properties can be tuned by the number, sequence and length of the individual polymer blocks [1,2]. Utilizing small-angle X-ray and neutron scattering in a wide temperature range, we investigate aqueous solutions of thermoresponsive tetrablock terpolymers having different sequences of hydrophilic, hydrophobic and thermoresponsive blocks. By fitting structural models, we gain insight into the shape and size of the micelles as well as their inner structure. Moreover, the gelation mechanism is deduced from the changes of the micellar structure and correlation at the gel point.

[1] A.P. Constantinou et al., Macromolecules 2018, 51, 7019
[2] A.P. Constantinou et al., Macromolecules 2025, 58, 9122

CPP 46.13 Thu 9:30 P5

Interfacial Dilational Rheology of Microgel Layer at the air-water interface — •Jana Sänger, Atieh Razavi, Regine von Klitzing, and Amin Rahimzadeh — Soft Matter at Interfaces, Institute for condensed Matter Physics, Technical University of Darmstadt, Hochschulstraße 8, 64289 Darmstadt, Germany

Interfacial tension and dilational interfacial rheology of Poly (N-Isoprpylacrylamide) (PNIPAM) microgel layer at air-water interfaces are characterized using pendant-drop techniques. Static interfacial tension was first measured with a drop shape analyser by fitting the droplet profile to the Young-Laplace equation. To probe the interfacial elasticity of microgel dispersions, a Profile Analysis Tensiometer (PAT-1) is employed to impose controlled harmonic oscillations on pendant drops with volumes of 10 μL and microgel concentrations between 0.1 wt% and 0.015 wt%. By using a Fourier transformation, the surface dilational modulus is determined, and the elasticity modulus is then identified as the real part of the surface dilational modulus. In order to remain within the linear range of the interfacial dilational elasticity, various amplitude ratios were systematically tested, and a maximum amplitude ratio of 6% was found. Our study shows that the elastic modulus is frequency-dependent. By increasing the frequency, an increasing elastic modulus is determined. Furthermore, we observe a shift of the maximum elasticity modulus towards the lower surface pressure values by increasing the frequency.

CPP 46.14 Thu 9:30 P5

Combined TGA-MS Analysis of Actively Aged Polymers for Assessing Recycling Potential — •Judith Bünte, Inga Ennen, Karsten Rott, and Andreas Hütten — Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany

Thermogravimetric analysis (TGA) combined with mass spectrometry (MS) provides a powerful, complementary approach for characterizing the thermal stability and degradation pathways of polymers subjected to accelerated (active) aging. In this study, aged polymer samples, representing materials encountered in post-consumer recycling streams, are analyzed using simultaneous TGA-MS to monitor mass-loss events and identify evolved gaseous species. These results demonstrate that combined TGA-MS analysis can reveal chemical and structural changes that are not easily evident from bulk mechanical or spectroscopic testing alone. The findings support more accurate assessments of polymer recyclability, highlight indicators of material downcycling, and inform optimization strategies for sorting, preprocessing, and reprocessing conditions. Ultimately, this work underscores the value of TGA-MS as a diagnostic tool for improving circular-economy approaches.

CPP 46.15 Thu 9:30 P5

Synthese und Reaktivität von Betti-Basen — •Alyona Nikulina — Mikluho-Maklaya Strasse, Moskau 117198

Diese Forschung konzentriert sich auf Naphthoxazine, eine wertvolle Gruppe von Verbindungen, die für ihre biologischen Aktivitäten bekannt sind wie antimikrobielle,antidiabetische und antidepressive Wirkungen sowie für ihr Potenzial in der Entwicklung von duroplastischen Polymeren. Die Synthese dieser Verbindungen beginnt häufig mit Betti-Basen, die Zwischenprodukte für die Bildung von kondensierten 1,3-Oxazinen darstellen.Um die notwendigen Betti-Basen zu erhalten, untersuchten wir zwei Syntheserouten. Eine Strategie war eine einfache Dreikomponenten-Reaktion von β-Naphthol, sekundären cyclischen Aminen und Aldehyden. Der andere Weg umfasste zunächst die Kondensation von 2-Hydroxy-1-naphthaldehyd mit Aminen und anschließend die Reduktion der resultierenden Iminiumsalze mit Natriumborhydrid. Nachfolgende Versuche, diese Basen durch Cyclisierung mit Standardreagenzien wie Silberoxid oder Kupferacetat in die Ziel-Naphthoxazine umzuwandeln, erwiesen sich als ineffizient und ergaben geringe Ausbeuten. Da bekannt ist, dass diese Cyclisierung die Bildung eines Iminiumsalzes beinhaltet, stellten wir die Hypothese auf, dass DIAD als wirksamer Katalysator wirken würde. Das Experiment nahm jedoch eine unerwartete Wendung: DIAD allein führte nicht zu den gewünschten Naphthoxazinen. Der entscheidende Moment kam, als wir ein katalytisches System aus Kupfer(I)-iodid und Cesiumcarbonat zugaben, das eine unvorhergesehene intramolekulare Umlagerung der Betti-Basen auslöste und stattdessen zu Diketon führte.

CPP 46.16 Thu 9:30 P5

Functional ZnPc-Polymer-Magnetic Nanocomposite Systems for Photodynamic Therapy — •Lungu Ion — Laboratory of Organic/Inorganic Materials for Optoelectronics, Institute of Applied Physics Moldova State University, 60 Al. Mateevici St., MD-2009, Chisinau, Republic of Moldova

Hybrid photosensitizing materials combining organic and magnetic components provide a promising route toward multifunctional systems for photodynamic therapy (PDT). In this work, we investigate the photophysical and magnetically induced processes in a series of functional zinc phthalocyanine (ZnPc) derivatives-ZnPc(COOH)4 and ZnPc(COOH)8 and their conjugates with dextran (Dx) and Fe3O4 nanoparticles. The systems were studied in DMSO/H2O (1:1) solutions using steady-state and time-resolved fluorescence and phosphorescence spectroscopy. All ZnPc-based compounds exhibit characteristic Q-band absorption (650-700 nm) and room-temperature phosphorescence with microsecond lifetimes, confirming efficient intersystem crossing (ISC). Dextran conjugation enhances fluorescence efficiency (ΦF = 2.37 %) and reduces aggregation, whereas Fe3O4 incorporation modifies the spin-orbit coupling, promoting magnetically assisted ISC and additional non-radiative channels. The triplet lifetimes vary between 1-9 μs, depending on molecular substitution and interfacial coupling. These results demonstrate that combining photoactive ZnPc cores with natural polymer matrices and magnetic nanoparticles enables control over excited-state dynamics and ROS generation for biomedical applications.

CPP 46.17 Thu 9:30 P5

Biopolymer-Templated Deposition of Hierarchical 3D-Structured Graphene Oxide/Gold Nanoparticle Hybrids for Surface-Enhanced Raman Scattering — •Yingjian Guo[1,2], Guangjiu Pan[2], Yusuf Bulut[1,2], Arno Jeromin[1], Thomas F. Keller[1], Andreas Stierle[1], Gergely Nemeth[3], Ferenc Borondics[3], Benedikt Sochor[1], sarathlal K. Vayali[1], Daniel Söderberg[4], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,4] — [1]DESY, Hamburg — [2]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [3]Synchrotron SOLEIL, Saint-Aubin, France — [4]Department of Fibre and Polymer Technology, KTH, 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 46.18 Thu 9:30 P5

Regulation of HUVEC Adhesion by Mechanical and Biochemical Tuning of PNIPAM Microgel Coatings — •Leonie Beer, Souraj Mandal, and Regine v. Klitzing — Soft Matter at Interfaces, Department of Physics, TU Darmstadt, Darmstadt 64289, Germany

A bioactive and stable interfacial layer favouring HUVEC cell adhesion is a key factor in artificial vascular network construction. This work investigates the impact of the mechanical and biochemical properties of PNIPAM microgel (MG) coatings on HUVEC cell adhesion and proliferation on 3D printed polymeric surfaces. MG stiffness can be varied based on cross-linking, and bioactivity can be imparted by functionalizing MG with RGD-based peptide mimicking extracellular matrix (ECM) ligands. HUVEC cell culture studies showed significant effects of MG stiffness on cell adhesion and proliferation, with further improvement due to biochemical functionalization. In addition, different spacers were used to enhance cell attachment and growth.

MG adhesion on different substrates was also evaluated, revealing significantly stronger adsorption on 3D-printed polymeric surfaces compared to inorganic substrates. AFM imaging confirmed the presence of firmly adhered MGs beneath the cells, demonstrating long-term coating integrity under biological conditions.

These results demonstrate that PNIPAM MG coatings provide a robust, tunable, and bioactive platform for controlling HUVEC behaviour and represent a promising strategy for endothelialization of 3D-printed vascular structures.

CPP 46.19 Thu 9:30 P5

Crystallization behavior of electron beam modified Polylactide acid (PLA) — •Regine Boldt[1], Elisabeth Hauschild[1], Michael Müller[1], and Markus Stommel[1,2] — [1]Leibniz Institut fuer Polymerforschung Dresden, Germany — [2]Dresden University of Technology, Germany

Polylactic acid (PLA) is a polymer synthesized from renewable raw materials. The properties of PLA are essentially determined by its chemical/physical structure, such as molar mass, molar mass distribution, D-isomer content, and the resulting morphology. The morphology can be influenced by modifying the molecular structure on the one hand, and by the process parameters during processing on the other. Since PLA crystallizes very slowly, high cooling rates, which occur in processing methods such as injection molding, usually result in amorphous components. In this work, we modified PLA using high-energy electrons in order to accelerate its crystallization without adding external additives. The resulting changes in crystallization kinetics were analyzed and correlated with the morphology after irradiation. The spherulite growth rates were determined quantitatively using hot stage experiments on a light microscope. The results show that electron-modified PLA exhibits substantially increased crystal growth rates, enabling significant reductions in cooling time during processing operations such as injection molding.

CPP 46.20 Thu 9:30 P5

Diffusion and stiffness characterization of photocrosslinked hydrogels to replicate biological tissues — •Lena Hilf[1], Dimitris Missirlis[1,2], and Kai Melde[1] — [1]Institute for Molecular Systems Engineering and Advanced Materials, Universität Heidelberg — [2]MPI for Medical Research, Heidelberg

Microphysiological systems (MPS), such as organs-on-a-chip, aiming to replicate the spatial arrangement of biological tissues found in vivo are in need of a reliable and replicable way to recreate the biophysical environment including topography and mechanical properties. One possible route is via selective photocrosslinking of hydrogel scaffolds, which can be performed in situ in microfluidic platforms.

However, we still lack reliable information about key properties of potential hydrogel candidates in these systems, which influence cell adhesion and spreading, as well as the uptake of media components.

In this work, we characterize the stiffness, mesh size and diffusion constant of a range of hydrogels created using photolithpgraphy. We employ both optical and mechanical approaches, taking into account the versatility of hydrogel responses to different measurement methods.

Our results together with cell proliferation assays allow for a more targeted choice of hydrogels to serve as artifical extracellular matrices in MPS.

CPP 46.21 Thu 9:30 P5

Characterization of bimodal PMMA-PDMS suspensions using light scattering — •Katharina Gaus and Joachim Wagner — University of Rostock, Rostock, Germany

Poly-dimethylsiloxane coated PMMA particles index matched in tetraline/decaline mixtures are well defined model systems for hard spheres with tunable particle size. Binary mixtures of these core-shell particles with slightly different sizes artificially increase the polydispersity of colloidal model systems preventing crystallization at large volume fractions and thus enabling the preparation of colloidal glasses. Using a priori knowledge of both species' topology, even in the limited range of wave vectors accessible with light scattering experiments, the reliable structural characterization of mixtures is possible. Hence, such binary mixtures are promising model systems for colloidal glasses.

CPP 46.22 Thu 9:30 P5

Cycles of buckling in gel phase giant unilamellar vesicles — •Azeline Hilaire, Antonio Stocco, Jean Farago, and Fabrice Thalmann — Institut Charles Sadron, Strasbourg, France

Buckling can be observed in giant unilamellar vesicles (GUVs) in gel phase, leading to shape deformations under external stress. Such deformations may offer functional advantages, particularly for inducing motion at low Reynolds numbers.

Recently, lipid-coated microbubbles were shown to exhibit directed motion through deformation cycles, suggesting a broader potential for soft interfaces to generate propulsion. Inspired by this, we investigate whether similar mechanisms can be used in isolated GUVs under cycles of deformation, with the goal of understanding and eventually triggering symmetry-breaking dynamics. We aim to use shape hysteresis for producing directed motion.

Gel-phase GUVs were fabricated via hydration method and characterized by their ability to transition between buckled and unbuckled states. We exposed these vesicles to cyclic fields using three distinct methods: (i) oscillatory shear flows, (ii) osmotic pressure, (iii) On/Off cycles of light applied with optical tweezers. In some of these cases, the membrane exhibited buckling.

Although directed motion has not yet been observed, the buckling response establishes a first result for future efforts to induce propulsion in vesicles. These preliminary results offer a first step towards exploring whether shape hysteresis in membranes could one day be used for active functions.

CPP 46.23 Thu 9:30 P5

Dynamics of trifunctional hybrid nanoparticle assemblies — •Thomas Dartige[1], Yinan Fan[2], Clément Marque[1], Ali Abou-Hassan[2], and Antonio Stocco[1] — [1]Institut Charles Sadron, Strasbourg, France — [2]Phenix Lab, Paris, France

Active colloids are colloidal systems able to consume energy to produce work, such as directed motion. Self-propulsion in micrometric particles can be achieved through surface asymmetries, using diffusiophoresis (via asymmetric catalytic properties) or thermophoresis (via asymmetric light absorption). However, the combining of several active properties into one single colloidal system remains poorly explored. In this work, we present a hybrid system synthesized by combining distinct nanoparticles, and investigate its ability to exhibit diffusiophoresis, thermophoresis, and respond to magnetic field gradients.

CPP 46.24 Thu 9:30 P5

Physics-Informed Neural Inference with Multilayer DWBA Modeling for Quantitative GISAXS — •Özüm Emre Asirim[1,2], Yufeng Zhai[1], Marina Tropmann-Frick[2], and Stephan V. Roth[1,3] — [1]Deutsches Elektronen-Synchrotron DESY FS-SMA Notkestr. 85 22607 Hamburg Germany — [2]HAW Hamburg Berliner Tor 7 20099 Hamburg Germany — [3]KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

Quantitative GISAXS analysis is often constrained by the complexity of multilayer scattering, film-nanoparticle coupling, and the limited availability of physically interpretable synthetic datasets for training modern inference models. We address these challenges with a physics-informed neural framework that integrates a compact multilayer DWBA formulation with a hybrid CNN-Transformer architecture. The forward model captures essential film and nanoparticle scattering through per-layer incoherent DWBA terms, normalized form factors, structure factors, and DWBA-based field enhancement, yielding a reduced and physically coherent parameter space suitable for inversion. Measurement variability is modeled through noise, detector effects, and the ability to generate time-series data for evolving structures. Leveraging this parameterization, the CNN-Transformer network jointly extracts local scattering motifs and long-range reciprocal-space correlations, enabling accurate recovery of film- and particle-level parameters. Validated through forward reconstruction using the same physics model, the workflow provides a fast, interpretable, and physically grounded solution for high-throughput GISAXS analysis.

CPP 46.25 Thu 9:30 P5

How Polymer Architecture Shapes the Phase Behavior of Polyelectrolyte Complex Coacervates — •Lena Tarrach, David Beyer, and Christian Holm — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

Polyelectrolyte (PE) complex coacervation is an associative liquid-liquid phase separation that can occur in mixtures of oppositely charged macromolecules. Although this phenomenon is widely studied, the effects of the polymer architecture on the phase behavior of PE complex coacervates have not been considered so far. To close this gap, in this contribution, coarse-grained molecular dynamics (MD) simulations with the ESPResSo software [1] are applied to calculate the phase diagram of branched PEs with varying numbers of arms but the same overall molecular weight. The slab method is used to establish the coexistence of the coacervate phase and the supernatant solution. The number of arms of the PEs is systematically increased to assess the influence of the PE topology on the phase behavior. The obtained phase diagrams are subsequently compared to theoretical phase diagrams calculated using the random phase approximation.

[1] Florian Weik, Rudolf Weeber, Kai Szuttor, Konrad Breitsprecher, Joost de Graaf, Michael Kuron, Jonas Landsgesell, Henri Menke, David Sean, and Christian Holm. ESPResSo 4.0 - an extensible software package for simulating soft matter systems. The European Physical Journal Special Topics, 227(14):1789-1816, 2019. doi:10.1140/epjst/e2019-800186-9.

CPP 46.26 Thu 9:30 P5

Self-assembled Micelles from Charged Block Copolymers: Insights from Small-Angle X-ray Scattering (SAXS) — •Yijun Zhao[1], Varvara Chrysostomou[2], Athanasios Skandalis[2], Stefano Da Vela[3], Stergios Pispas[2], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]Theoretical and Physical Chemistry Institute, NHRF, Athens, Greece — [3]EMBL at DESY, Hamburg, Germany

Block copolymer micelles have been widely studied due to their ability to load drugs. Positively charged micelles have been proposed to complex DNA, enabling efficient gene therapy. To achieve highly tunable morphology, self-assembled micelles from the diblock copolymers PDMAEMA-b-PLMA and the triblock terpolymers PDMAEMA-b-PLMA-b-POEGMA are investigated in aqueous solution [1]. Here, PDMAEMA stands for the weak polycation poly(2-(dimethylamino)ethyl methacrylate), PLMA for the hydrophobic, but soft poly(lauryl methacrylate), and POEGMA for the hydrophilic poly(oligo(ethylene glycol) methacrylate). Small-angle X-ray scattering (SAXS) on dilute aqueous solutions revealed that PDMAEMA-b-PLMA forms ellipsoidal core-shell micelles, with their size and inner structure depending on temperature and the pH value. For the triblock terpolymers, the micellar structures depend strongly on the block lengths.

[1] V. Chrysostomou et al., J. Polym. Sci. 63 1684-1694 (2025).

CPP 46.27 Thu 9:30 P5

Pump-probe spectroscopy on the polyelectrolyte donor polymer PTHS for solar cell applications — •Mick Gindorf[1], Anna Köhler[1], Christopher Vogt[2], and Johannes C. Brendel[2] — [1]Chair of Soft Matter Optoelectronics, University of Bayreuth — [2]Chair of Macromolecular Chemistry I, University of Bayreuth

Poly(3-hexylthiophene) (P3HT) is a well-researched donor polymer for application in organic solar cells (OSCs). Side chain modification of P3HT with sulfonate groups yields PTHS, a polyelectrolytic donor polymer with high hole transport mobility [1]. This polyelectrolyte possesses two key advantages: Firstly, exchange of the cationic counter ions enables insolubilization of the donor layer, allowing simple fabrication of donor-acceptor bilayer systems by sequential spin coating with a wide variety of acceptors, including both fullerene and non-fullerene acceptors (NFAs). Secondly, adjusting the counter ion composition enables tuning of the donor energy level and thereby the donor-acceptor energy level offset (E_{off}), which is critical for achieving high open circuit voltages (V_{oc}). These properties make PTHS an ideal model system for the investigation of exciton dissociation in OSCs with spectroscopic techniques, including time-resolved transient absorption spectroscopy. Probing the exciton dissociation dynamics as a function of E_{off} on a picosecond timescale in different donor-acceptor systems yields valuable insights into the energetic and entropic contributions that help overcome the exciton binding energy in OSCs.

1) Brendel, J. et al. Chem. Mater. 2014, 26, 6, 1992-1998

CPP 46.28 Thu 9:30 P5

PEDOT Molecular Imprinting in PEDOT:PSS/PDADMA Layer-by-Layer Films — •Martin Hunger, Muhammad Khurram, and Christiane A. Helm — martin.hunger@uni-greifswald.de

PPEDOT:PSS films are widely used because they offer high conductivity & tunable electro-optical properties. We prepare PEDOT:PSS films with a thickness of up to 150 nm using Layer-by-Layer assembly. We vary the preparation conditions: flow cell, dip coating, PEDOT:PSS concentration in solution, and rinsing steps. Whenever PDADMA is the top layer, UV-vis-IR absorption spectroscopy shows that there is significantly less PEDOT in the films than when PEDOT:PSS is the top layer. Films prepared using the flow cell have the highest electrical conductivity (approx. 200 kS/m) with PEDOT:PSS. When PEDOT is the top layer, conductivity is reduced by a factor of 100. The conductivity of films prepared with dip coating with PEDOT:PSS as the top layer is one order of magnitude lower or more. When PDADMA is the top layer, conductivity drops by an additional 4 to 5 orders of magnitude. Thus, during assembly, PEDOT can be selectively removed and subsequently rebound to the film, leaving behind well-defined molecular cavities that preserve their shape and enable reconstruction of percolative pathways.

CPP 46.29 Thu 9:30 P5

PDADMA/PSS Multilayer Buildup in NaBr Solution: Vertical PSS Diffusion and Unusual Growth — •Per-Ole Hilken, Issam Assi, and Christiane A. Helm — Institute of Physics, University of Greifswald, Germany

Polyelectrolyte multilayers form by sequential adsorption of oppositely charged polyelectrolytes. The interfaces between the adsorption layers are fuzzy; in the exponential growth regime of PDADMA/PSS (poly(diallyldimethylammonium)/polystyrene sulfonate) multilayers PSS diffuses vertically through the film. We determine its vertical diffusion coefficient D_{PSS} using a quartz crystal microbalance with dissipation (QCM-D). The scaling laws for D_{PSS} in dependence of the NaBr concentration are similar to those found with NaCl in the deposition solution (Sill et al., Macromolecules 2025), however, the diffusion coefficient is one to two orders of magnitude larger. The dependence on PSS molecular weight M_{PSS} is qualitatively the same as with NaCl in the deposition solution: Polymer diffusion dominates multilayer build-up when $M_{PSS} < 76$ kDa.; at larger M_{PSS}, site diffusion dominates; i.e. diffusion of charged repeat units with their counterions. For polyelectrolyte multilayers in the non-exponential growth regimes it is well known and also found with that an increase in the salt concentration leads to thicker multilayers. This is not the case if the NaBr concentration exceeds ≈ 0.6 M; additionally, film stability becomes an issue. To understand the unusual behavior, the dissipation during film build-up is quantified. The surface topography is investigated with AFM.

CPP 46.30 Thu 9:30 P5

Structural influences on nonlinear optical activity in the heterocubane family — •Alexander Kapp and Simone Sanna — alexander.kapp@pysik.uni-giessen.de

Recent progress in the study of molecular clusters with extreme nonlinear optical response has highlighted their potential for coherent broadband light generation. To extend the library of suitable candidate materials, we investigate the linear and nonlinear optical properties of a family of heterocubanes with the general formula $[(RM)_4Pn_4]$, where M = C, Si, Ge, Sn, Pn = N, P, As, Sb, Bi, and R = H, Me, Ph. Using *ab initio* density functional theory, we analyze their structural and electronic characteristics, including optimized geometries, symmetry features, band gaps on different theoretical levels and shape of the HOMO–LUMO orbitals. Both the linear and the nonlinear (SHG) optical responses of all systems are computed using the Yambo code. Clear trends emerge that link the optical activity to the choice of pnictogen, tetrel, and substituent. These findings help identify promising candidates for nonlinear optical applications and contribute to a deeper understanding of structure–property relations in heterocubane materials.

CPP 46.31 Thu 9:30 P5

A micellar solution from thermoresponsive block copolymers during pressure jumps — •Yandong Wang[1], Geethu P. Meledam[1], Leonardo Chiappisi[2], Cristiane Henschel[3], André Laschewsky[3,4], Alfons Schulte[5], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]ILL, Grenoble, France — [3]Universität Potsdam, Germany — [4]Fraunhofer IAP, Potsdam-Golm, Germany —

[5]University of Central Florida, Orlando, U.S.A.

The diblock copolymer PMMA-b-PNIPAM, consisting of a hydrophobic poly(methyl methacrylate) and a thermoresponsive poly(N-isopropylacrylamide) block, forms core-shell micelles in dilute aqueous solution at atmospheric temperature. These micelles aggregate upon heating or applying pressure. Previous studies have shown that the micellar shell remains hydrated in the two-phase region under high pressure, in contrast to the strongly dehydrated micelles observed in the two-phase region at atmospheric pressure [1]. In this work, we analyzed the micellar transition kinetics during rapid pressure jumps using time-resolved small-angle neutron scattering (SANS). The system was driven from the one-phase region into the two-phase region at target pressures in both low- and high-pressure regimes.
[1] P. A. Alvarez Herrera et al., Macromolecules 2024, 57, 10263.

CPP 46.32 Thu 9:30 P5

Photoresponsive Interfacial Behavior of Hybrid Photosensitizer-Surfactant Mixtures — •Phat Tan Pham[1], Julius Gemen[2], Frank Glorius[2], and Björn Braunschweig[1] — [1]Universität Münster, Institut für Physikalische Chemie, Corrensstr. 28/30, 48149 Münster — [2]University of Münster, Organisch-Chemisches Institut, Corrensstraße 40, 48149 Münster

Fluid interfaces that adapt to external triggers such as light or temperature are of great interest for driving changes in soft matter systems like foams and emulsions. Arylazopyrazoles (AAPs), as photo-responsive surfactants, can control surface tension and molecular organization at air-water interfaces through E/Z photoisomerization. However, light-induced switching of AAP derivatives is typically limited to UV and green light. To overcome this, we combined AAP with the water-soluble photosensitizer resazurin (Rez) and achieved pronounced interfacial changes under 625 nm red-light irradiation. By tuning the AAP/Rez molar ratio, we further introduced history-dependent, quasi-adaptive changes in surface tension and molecular structure. The latter was examined in situ with surface tensiometry and vibrational sum-frequency generation (SFG) when the samples where irradiated at 365, 520, or 625 nm. We propose that red-light activation occurs at the interface, through photoexcited Rez moieties at 625 nm and subsequent intersystem crossing to adjacent interfacial AAP molecules. These results demonstrate a new strategy to extend the optical control of photo-responsive surfactants into the red-light region.

CPP 46.33 Thu 9:30 P5

Thermoresponsive Microgel Membrane for applications in an Electrochemical Device — •Aditi Gujare[1], Stefanie Uredat[2], Jonas Runge[2], Domenico Truzzolillo[1], Julian Oberdisse[1], and Thomas Hellweg[2] — [1]Soft Matter Physics Team, Laboratoire Charles Coulomb, University of Montpellier, Montpellier, France — [2]Physical and Biophysical Chemistry, Bielefeld University, Bielefeld, Germany

Microgels based on NIPAM are thermoresponsive with a volume phase transition temperature (VPTT) of 33°C. The VPTT has been observed to shift by copolymerizing these microgels with comonomers such as N-hydroxymethyl acrylamide (HMAM).[1] Different sets of copolymers have been tested, NIPAM-co-HMAM and NIPMAM-co-HMAM. These microgels have been observed to have a VPTT up to 60°C. The copolymer microgels based on the comonomer HMAM has an alcohol group, making it prone to condensation at high temperatures (above 90°C) resulting in formation of a membrane. These thermoresponsive, chemically crosslinked membranes have been prepared by dropcasting and crosslinking at 100°C. Such membranes can be prepared in a range of thickness, of 30-800 μm. The resistance of these membranes of different thickness, comonomer content, and at different temperatures are being tested. Resistance measurements at room temperatures show that thicker membranes are more resistive in a certain concentration of an electrolyte. [1]Gujare,Uredat,Runge,Morgenstern,Truzzolillo,Hellweg,Oberdisse, Langmuir 2025, 41, 45, 30442

CPP 46.34 Thu 9:30 P5

Correlating molecular properties of tetraphenylethylene substituted tetraphenyl heteoadamantanes to nonlinear optical activity — •Eva Westenfelder Gil and Simone Sanna — Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Germany

Recent studies have demonstrated white light generation from molecular clusters with adamantane-like cores and various substituents [1,2]. Subsequent investigations on isolated molecules revealed correlations of the structural, electronic and optical properties [3]. Building on this foundation, we focus here on further investigating structural, electronic, and (nonlinear) optical properties from first principles for isolated molecules with modified cores. In this contribution, we report on $[(PhSn)_3(TPESi)S_6]$ and $[(PhSn)_3(TPESi)Se_6]$ clusters, which are modeled within density functional theory. Distinct changes in the spectral signatures can be observed. The presented results expand on theoretical foundations for the design of tailored nonlinear optical sources.
[1] N. W. Rosemann *et al*, Science 2016, 352, 1301
[2] N. W. Rosemann *et al*, J. Am. Chem. Soc. 2016, 138, 50, 16224-16227
[3] F. Ziese *et al*, 2024. J. Phys. Chem. A 128, 8360-8372

CPP 46.35 Thu 9:30 P5

Modeling Structural and Electronic Properties of Functional Organic Molecules — •Linda Düren and Simone Sanna — Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Germany

In this work, various organic molecules with the general composition $[(RT)_4E_6]$ are investigated using density functional theory (DFT) to model their structural, electronic, and optical properties. Ground-state geometries and energies, as well as the frequency-dependent optical parameters, are calculated for the isolated clusters. The study includes *tetraphenyladamantane* and its halogenated derivatives, as well as other heteroadamantanes with a heterogeneous ligand field of the type $(MeC)(CH_2)_3(PhSn)E_3$ with E = S, Se, Te, CH_2.

The theoretical results provide insights into the relationship between molecular structure and optical behavior, building on previous studies of nonlinear optical responses in organotetrel and (hetero)adamantane-type clusters [1] and amorphous molecular materials for directed supercontinuum generation [2]. The results are compared with experimental data where available and demonstrate the potential of these classes of molecules for applications in optics.
[1] Ziese et al., *J. Phys. Chem. A* **128**, 8360 (2024)
[2] Dehnen et al., *ChemPhotoChem* **5**, 1032 (2021)

CPP 46.36 Thu 9:30 P5

Tuning PNIPAM Phase Transition and Interfacial Structures — •Zugeng Cong, Michael Hardt, and Björn Braunschweig — University of Münster, Institute of Physical Chemistry, Münster, Germany

In this work, we aim to introduce the concept of a self-regulating negative-feedback system in which an exothermic photochemical process would be coupled to the thermo-responsive polymer PNIPAM. In such a scheme, reaction-generated heat would raise the solution temperature, trigger PNIPAM collapse, increase turbidity, and thereby limit light penetration—providing an intrinsic mechanism to suppress further heat generation. For that, we characterize the PNIPAM phase transition through temperature-dependent turbidity measurements while varying SDS and NaCl concentrations as well as the water-ethanol co-solvent composition. To elucidate interfacial contributions, surface-specific sum-frequency generation (SFG) spectroscopy is used to probe adsorption layers at the air-water interface, taken as a model for micellar environments. These measurements reveal how surfactant loading, solvent composition, and electrolyte concentration reorganize interfacial structures below and above the PNIPAM phase-transition temperature. This provides the physicochemical basis required for designing a feedback-controlled photochemical soft matter system.

CPP 46.37 Thu 9:30 P5

Quasi-elastic neutron scattering of perdeuterated poly(N-isopropylacrylamide) and hydration changes across the demixing transition — •Alfons Schulte[1], Eric Rende[1], Marcell Wolf[2], Thomas Müller[3], Dirk Schanzenbach[4], Andre Laschewsky[4,5], and Christine M. Papadakis[6] — [1]Department of Physics and College of Optics and Photonics, University of Central Florida, Orlando, U.S.A. — [2]Heinz Maier-Leibnitz Zentrum (MLZ), TUM, Garching, Germany — [3]FZ Jülich, JCNS at MLZ, Garching, Germany — [4]Institut für Chemie, Universität Potsdam, Potsdam-Golm, Germany — [5]Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm, Germany — [6]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany

We investigate the hydration dynamics of perdeuterated poly(N- isopropylacrylamide) (PNIPAM-d10) to elucidate the molecular mechanism of its demixing transition. Quasi-elastic neutron scattering (QENS) and Raman spectroscopy were measured in a 25 wt% PNIPAM-d10 aqueous solution over the temperature range from 298 to 325 K. There is a significant upward shift in the cloud point by about 4 degrees. Deuteration suppresses incoherent scattering from the polymer, allowing a clear view of hydration water dynamics. The dynamic susceptibilities reveal the relaxation processes for bulk and bound water, with the bound fraction decreasing sharply near the transition. The relaxation times of hydration water are consistently lower than in the protiated polymer, indicating faster local dynamics. Raman spectra show abrupt C-D band frequency shifts at the transition, reflecting side-group dehydration.

CPP 46.38 Thu 9:30 P5

Thermoresponsive Microgels with hydrophilic Monomers — •Stefanie Uredat[1], Aditi Gujare[2], Jonas Runge[1], Domenico Truzzolillo[2], Julian Oberdisse[2], and Thomas Hellweg[1] — [1]Physical and Biophysical Chemistry, University Bielefeld, Bielefeld, Germany — [2]Laboratoire Charles Coulomb (L2C), University of Montpellier, CNRS, Montpellier, France.

To develop fully smart membranes for use in low-temperature fuel cells operating at around 80-90 °C it is essential to achieve a high volume phase transition temperature (VPTT) within this range. To reach these high VPTTs, new monomers are required for microgel synthesis. The most common and researched monomers have a VPTT around the human body temperature [1]. To rise the VPTT we increased the hydrophilicity of the monomers by adding a hydroxy group to the well-known NIPAM and got HIPAM (N-(2-hydroxyisopropyl)acrylamide).

To tune the VPTT to higher Temperatures a series of microgels with two different main monomers (NIPAM and NIPMAM) with different contents of HIPAM as comonomer were synthesised. The microgels were observed by Dynamic Light Scattering and AFM. With higher HIPAM content the VPTT of the microgels increases and widens. We also observe a jump in size with increasing hydrophilic monomer content. We also investigated a second hydrophilic monomer N-(hydroxymethyl)acrylamide (HMAM). [2]

[1] Uredat, Runge, Gujare, PCCP, 2024, 2732. [2] Gujare, Uredat, LANGMUIR 2025, 41, 45, 30442 [3] The authors acknowledge funding from the DFG (505656154) and ANR (ANR-22-CE92-0052-01)

CPP 46.39 Thu 9:30 P5

The phase transition of perdeuterated thermoresponsive polymers — •Chenrui Ding[1], Kuno Schwärzer[2], Alfons Schulte[3], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]JCNS-1, FZ Jülich GmbH, Germany — [3]University of Central Florida, Department of Physics and College of Optics and Photonics, Orlando, U.S.A.

The interaction of thermoresponsive polymers with water has been amply studied with respect to the cloud point temperature and the latent heat at the transition, using, among others, turbidimetry and differential scanning calorimetry (DSC) [1]. New information on the polymer-water interaction can be gained using perdeuterated polymers. We present results on poly(N-isopropyl acrylamide) (PNIPAM) and poly(N-isopropyl methacrylamide) (PNIPMAM) and their perdeuterated versions in aqueous solution as a function of polymer concentration and establish the transition behavior.

1. C.-H. Ko, C. M. Papadakis et al., Macromolecules 53, 6816 (2020)

CPP 46.40 Thu 9:30 P5

Steel Mesh-Supported SNW-1/CsPbBr3 Nanocomposite: Photocatalyst for Sustainable Ammonia Production — •Negin Khosroshahi and Vahid Safarifard — Iran University of Science and Technology, Tehran 16846-13114, Iran

The conversion of solar energy into chemical energy through photocatalysis is an important field of interest in green energy generation and environmental improvement [1]. Nevertheless, its effectiveness currently falls short of expectations, primarily due to the issue of charge recombination. To address this challenge, the photocatalytic effect has become an optimistic approach for enhancing processes [2]. In this research, we have developed a Steel Mesh-Supported SNW-1/CsPbBr3 nanocomposite by combining covalent-organic frameworks with metal halide perovskite. To gauge their effectiveness, the heterostructure was assessed by employing multiple characterization methods including XRD, IR, FESEM, DRS, EDX, VSM, PL, EIS, Zeta, and BET. After the composite's preparation and characterization, we examined its photocatalytic activity in nitrogen reduction. The SNW-1/MHP/Steel mesh nanocomposite exhibited exceptional performance in ammonia generation. These findings suggest that the SNW-1/MHP/Steel mesh nanocomposite holds promise as an environmentally friendly and cost-effective photocatalyst, capable of addressing the challenges of sustainable ammonia production. This study presents a promising method for identifying effective photocatalytic materials using mesh substrates to address environmental concerns.

CPP 46.41 Thu 9:30 P5

Engineering MOF@MOF Heterojunction for Photocatalytic N2 Reduction to NH3 — •Maedeh Atoufi Kashani, Negin Khosroshahi, and Vahid Safarifard — Iran university of science and technology, Tehran, Iran

Photocatalytic nitrogen fixation is a promising green alternative to the Haber-Bosch process, but cobalt-based MOFs typically suffer from poor stability in water. Here, two Co-terephthalate frameworks were synthesized via solvothermal routes: MOF-71 from Co(NO3)3.6H2O and ultrathin Co-BDC nanosheets from CoCl2.6H2O in the presence of triethylamine, water, and ethanol. Both materials showed high phase purity and strong visible-light absorption. To improve the limited stability of Co-BDC, a Ce-based MOF overlayer was constructed on Co-BDC and MOF-71, forming a Ce-Co MOF-on-MOF composite. The Ce shell enhanced water stability, facilitated charge separation, and promoted N2 activation at the heterointerface. As a result, the Ce-Co-BDC composite delivered markedly higher ammonia production and durability than pristine Co-BDC. This work highlights the critical roles of precursor chemistry and Ce-Co interfacial engineering in developing robust MOF photocatalysts for solar-driven nitrogen fixation. [1] S. Nabi, M.M. Bhat, A. Hamid, A.Y. Bhat, A.U. Bashir, Q. Jan, P.P. Ingole, M. Bayati, M.A.J.A.S.S. Bhat, (2025) e00112. [2] G. Song, Y. Shi, B. Yang, Y. Yang, H.J.I.C. Pang, 64 (2025) 6265-6274.

CPP 46.42 Thu 9:30 P5

Structural Insights into Supported Ionic Liquid Phases — •Yufei Wu[1], Julius Schlüter[2], Chandan K. Das[3], Zhuo Chen[1], Alexis Bordet[1], Maria Fyta[3], and Thomas Wiegand[1,2] — [1]Max Planck Institute for Chemical Energy Conversion, Mulheim an der Ruhr, Germany — [2]Institute of Technical and Macromolecular Chemistry, RWTH Aachen University, Aachen, Germany — [3]Computational Biotechnology, RWTH Aachen University, Aachen, Germany

Metal nanoparticles supported on molecularly modified surfaces (MMSs) offer significant potential for the development of advanced materials chemistry, particularly in catalysis. In this work, we focus on supported ionic liquid phases (SILPs) as a representative class of MMS materials. The SILP material was synthesized by functionalizing an amorphous silica surface with a layer of phosphonium-based ionic liquid (IL) covalently bound to the silica. The structural features of the SILP, specifically the conformation of the phosphonium IL cations, were characterized using magic-angle spinning (MAS) solid-state NMR spectroscopy. To complement the experimental findings, all-atom molecular dynamics (MD) simulations were performed on IL-modified silica surfaces. These simulations provided atomic-level insights into the structural organization and conformational dynamics of the IL molecules in the SILP materials. This combined approach paves the groundwork for future studies aimed at realizing SILP materials as efficient catalytic templates.

CPP 46.43 Thu 9:30 P5

Towards stable passivation layers on III-V-semiconductor nanowires for photoelectrochemical water splitting applications — •Chris Yannic Bohlemann, Pavithira Manoharan, Sahar Shekarabi, Peter Kleinschmidt, Thomas Hannappel, and Juliane Koch — Technische Universität Ilmenau, Fundermentals of Energy Materials, Ilmenau, Germany

The production of green hydrogen is expected to play a crucial role in achieving a sustainable, climate-neutral economy. Although III-V semiconductors offer record solar-to-hydrogen conversion efficiencies, the large-scale deployment is limited by the scarcity of the required materials. III-V nanowires (NWs) are a promising approach, as they require less material than planar films, and exhibit an enhanced optical absorption, as well as benefit from a high surface-to-volume ratio [1].

However, the instability of III-V materials in aqueous electrolytes leads to rapid corrosion and short lifetimes of photoelectrodes. To address this limitation, we investigated the growth behavior, electrical properties, and corrosion stability of GaAsP NWs and subsequently passivated with GaP(N) shells grown via metal-organic vapor-phase epitaxy. Scanning electron microscopy was used to examine the growth quality, crystal orientation, defect structures, and degradation before and after extended operation under water splitting conditions. Our results demonstrate that the application of a GaP(N) passivation layer significantly enhances the structural integrity and durability of the NWs during continuous photoelectrochemical water splitting.

[1] J. Koch et al., Adv. Energ. Sust. Res. e202500156, 2025.

CPP 46.44 Thu 9:30 P5

A Bottom-Up Coarse-Grained Model of Nanoparticles Decorated with Oppositely Solvent-Responsive Diblock Copolymers for Reversible Self-Assembly — •Daniel Otschkowski and Arash Nikoubashman — Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

Polymer-grafted nanoparticles (PGNPs) combine the optical, magnetic, or electronic functionality of inorganic cores with the elasticity and responsiveness of polymer chains. This hybrid character offers multiple, orthogonal design parameters for controlling the structure and properties of PGNP-based materials. In this work, we study spherical NPs grafted with amphiphilic diblock copolymers composed of two blocks with opposing solvent affinities, enabling reversible transitions between assembly and disassembly states. In the assembly state, the inner polymer block is solvophilic while the outer block is solvophobic, thus collapsing into attractive patches; in the disassembly state, the inner block forms a dense polymer shell which is surrounded by a stabilizing hydrophilic polymer corona. To access device-relevant time and length scales, we develop a bottom-up coarse-grained (CG) model, where we describe the PGNPs in the assembly state as particles with flexible, spring-tethered patches. Smoothly varying the effective interactions allow the CG model to reproduce the continuous transition between both states. This approach enables efficient simulation of large PGNP systems and provides insight into their reversible, stimuli-responsive behavior.

CPP 46.45 Thu 9:30 P5

Organic cathodes based on polyaniline and cellulose for aqueous Zn-ion batteries — •Ramsha Wasi Khan[1], Meriem Boudjenane[1], Gilles Wittmann[1], Xaver Brehms[2], Simon Schraad[3], Xinyu Jiang[3], Stephan V. Roth[3], and Lucas P. Kreuzer[1] — [1]Heinz Maier Leibnitz Zentrum (MLZ), TUM, Garching, Germany — [2]CEA, Grenoble, France — [3]DESY, Hamburg, Germany

Aqueous zinc-ion batteries are promising candidates for a non-toxic and safer alternative to lithium-ion batteries, where organic cathodes provide distinct advantages of sustainability, tunability and mechanical flexibility. In this work, we investigate the role of polyaniline (PANI) as an organic cathode material, motivated by its high theoretical capacity, reversible redox chemistry, and intrinsic electrical conductivity. To enhance stability against humidity-induced degradation, cellulose derivatives are employed as green binders, enabling regulation of water uptake and improved mechanical stability. Comprehensive multiscale characterization is conducted to optimize the electrochemical performance and structural integrity of PANI-based cathodes, as well as understand the morphological changes and nanoscale water dynamics under humidity. Advanced techniques such as cyclic voltammetry, scanning electron microscopy (SEM), and quasi-elastic neutron scattering (QENS) are used to support this analysis. It was observed that the use of composite cellulose films as a binder with an optimized composition effectively triples the current density and improves peak reproducibility as well as the water uptake behaviour of the film.

CPP 46.46 Thu 9:30 P5

Integration of Ag_2S nanocrystals into flexible polymer matrices — •Dolores García de Viedma Guerra, Peijiang Wang, and Beatriz Hernández Juárez — Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid E-28049, Spain

A broad range of modern optical technologies, for instance flexible photonics, require luminophores to be embedded within mechanically versatile host materials [1]. Usually, transferring nanocrystals from colloidal dispersions into polymer networks alters their physicochemical environment, which promotes surface traps and can thus signify a loss in photoluminescence [2].

In this work we investigate Ag_2S nanocrystals integrated into flexible polymer matrices with the goal of preserving their NIR response. We assess nanocrystal dispersion and spatial homogeneity, and probe their optical performance under 808 nm laser excitation via photoluminescence measurements and infrared spectroscopy, while NIR imaging maps emission uniformity. The results yield bright, uniform nanocrystal-polymer composites suitable for optoelectronic integration.

[1] Gordillo, H. et al. "Polymer/QDs Nanocomposites for Waveguiding Applications".*Journal of Nanomaterials* 2012, 960201, 2012.

[2] Marcus Jones et al. "Signatures of Exciton Dynamics and Carrier Trapping in the Time-Resolved Photoluminescence of Colloidal CdSe Nanocrystals". *The Journal of Physical Chemistry* C 2009, 113 (43), 18632-18642.

CPP 46.47 Thu 9:30 P5

Exploring the length limit for freestanding electrodeposited Ni nanowires — •Anneliese Wirth and Karin Leistner — Chemnitz University of Technology, Chemnitz 09107, Germany

Magnetic nanowire arrays are of interest from a fundamental and application point of view due to the shape anisotropy and high surface-to-volume ratio. This can be advantageous for 3D memory devices, micro-hard magnets and catalysis. The goal of this project is to obtain freestanding Ni nanowire arrays in order to functionalize their surface and possibly apply electrolytic gating strategies for 3D magneto-ionic materials in the future.[1] The Ni nanowire synthesis is performed by electrodepositing Ni into aluminum oxide membranes that serve as templates. Afterwards, the template is removed via dissolution of the aluminum oxide to achieve freestanding nanowires. For nanowires with high aspect ratio, this step usually leads to the collapse of the wires into agglomerated bundles.[2] This causes the loss of the nanowires' perpendicular alignment to the substrate. We show an optimized synthesis that avoids the collapse of nanowires with high aspect ratio in a large-scale array with a total size of around 0.5 cm^2. The deposition time during the electrodeposition is varied to obtain nanowires reaching up to more than 10 μm length while the diameter is fixed to 200 nm. Scanning electron microscopy indicates that the freestanding nature is related to irregularities of the nanowires which are introduced by the specific template geometry and lead to the stabilization of the array. [1] M. Nichterwitz et. al, ACS Mater. Au 2024, 4, 55. [2] N. Winkler et. al, J. Mater. Chem. 2012, 22, 16627.

CPP 46.48 Thu 9:30 P5

Structure and Morphology Investigations of Perovskite Nanocrystal Film — •Azam Davoodabadifarahani[1,2], Thomas Baier[1], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]University of Applied Sciences, Munich, Germany

In recent years, perovskite quantum dot solar cells with the ABX3 structure have shown great promise due to their high power conversion efficiency (PCE), high photoluminescence quantum yield (PLQY) and narrow photoluminescence (PL) peak. Within the presented work, the active layer consists of PQD thin films based on CsPbI3 and FAPbI3, which exhibit high photoelectric performance. However, CsPbI3 has a challenge with phase instability and FAPbI3 suffers from weak structural stability. To balance the performance and stability of the active layer, FAxCs1-xPbI3 PQDs are employed as the light-absorbing layer. The samples are evaluated using various optical and structural characterization techniques, such as PL spectroscopy, scanning electron microscopy (SEM), X-ray diffraction (XRD) and grazing incidence x-ray scattering (GIXS) to observe the influence of the synthesis process, temperature, and deposition techniques on the crystal size, orientation, phase, and stability, all of which determine the external quantum efficiency and optical performance.

CPP 46.49 Thu 9:30 P5

Surface-induced morphology and in-plane order in thin films of polydiketopyrrolopyrroles — •Anton Sinner and Oleksandr Dolynchuk — Martin Luther University Halle-Wittenberg, Germany

Board-like conjugated polymers are of particular interest in the context of surface-induced ordering because they often exhibit a preferred out-of-plane molecular orientation in thin films. Recent studies of ordering in conjugated polymer films have found that the free surface induces the formation of sanidic liquid crystalline (LC) mesophases with out-of-plane, smectic-like positional order between polymer chains. However, the question of whether the surface influences the in-plane order between polymer chains during ordering remained open. Here, we use atomic force microscopy to investigate the surface morphology and nanoscale structure formed on the surface of polydiketopyrrolopyrrole (PDPP) films after slow cooling and ordering from the melt. We find that the surface morphology consists of disc-like crystallites with diameters roughly equivalent to the polymer contour length and heights equivalent to several out-of-plane polymer layers. Thus, the observed LC morphology is consistent with the earlier study of out-of-plane molecular order. On a larger scale, multiple LC discs arrange into string-like morphologies, suggesting the existence of orientational order among them. Quantitative analysis of the surface morphology allows for calculating a distance-dependent orientation correlation function for six-fold symmetry, which indicates the presence of quasi-long-range order on the surface of PDPP films.

CPP 46.50 Thu 9:30 P5

Investigation of structure and transport properties in redox-active polymers — •Laura Hölzer[1] and Diddo Diddens[2] — [1]Institut für Physikalische Chemie, Universität Münster, 48149 Münster, Germany — [2]Helmholtz Institute Münster, Forschungszentrum Jülich GmbH, 48149 Münster, Germany

Organic radical batteries are seen as an alternative to traditional lithium-ion batteries. Their advantages include fast charge and discharge processes, and mechanical flexibility. However, high power densities are required for their application in the Internet of Things. To achieve this, good charge transport is essential. This transport mechanism is guided by two factors: the movement of electrons along the polymer, which is dictated by its structure, and the compensation of charge by counterions, which affects their mobility. The focus here is on a cathode material consisting of a redox-active polymer such as poly(2,2,6,6-tetramethylpiperidinyloxy-4-ylmethacrylate) (PTMA), which is in contact with a solvent. Classical molecular dynamics simulations of a PTMA cathode model are carried out. These provide insights into the structural properties and dynamics of charge transport. An outlook on the behaviour at interfaces around the cathode is given.

CPP 46.51 Thu 9:30 P5

Ex-Situ Investigation of Latex Deformation — •Simon Schraad[1,2], Shuxian Xiong[1,2], Helder Marques Salvador[3], Benedikt Sochor[1], Sarathlal Koyiloth Vayalil[1,4], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,5] — [1]DESY, Hamburg, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [3]CPP, Venlo/Poing, Netherlands/Germany — [4]UPES, India — [5]KTH, Department of Fibre and Polymer Technology, Stockholm, Sweden

Colloidal polymer latexes are used in ink-jet printing to form a pigment stabilizing layer on top of the cellulose layer. The latex film formation (LFF) is influenced by humidity, temperature, minimum film formation temperature (MFFT), and glass transition temperature (T_g). Exceeding MFFT polymer colloids begin to deform and further heating above the T_g polymers interdiffuse and coalesce into a homogeneous coating layer. Here we investigate cellulose nanofibrils (CNF) thin films coated with polystyrene colloids (diameters ranging from 100 to 500 nm) and commercially available polymeric colloids with different MFFT (Neocryl A639 and A1127). The samples were prepared by spray coating at temperatures below and above their T_g. Scanning electron microscopy revealed the size and shape of the colloids. Grazing incidence small angle scattering data shows contributions of spherical form factors from the colloids with respective diameters, which changes upon heating. 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 46.52 Thu 9:30 P5

A DFTB Pseudoatom-Based Fragmentation Strategy — •Kevin Mächtel — Karlsruher Institut für Technologie, Institut für Physikalische Chemie, Karlsruhe, Germany

Theoretical investigations of charge transport mechanisms in large molecular systems often rely on efficient fragmentation strategies, to reduce computational costs. In conventional approaches, link atom fragmentation has been used for this purpose, but pseudoatom approaches offer a more versatile alternative. They enable more efficient molecular fragmentation, simplifying the overall fragmentation process. In this study, we develop a novel density functional tight-binding pseudoatom fragmentation scheme for complex molecular systems. We tested our approach on 9,10-di(quinolin-6-yl)phenanthrene and demonstrated strong agreement with the established link atom method.

CPP 46.53 Thu 9:30 P5

Benchmarking the Transferability of Machine Learning Interatomic Potentials for Polymers — •Mirko Fischer and Andreas Heuer — Institute for Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster

Machine Learning Interatomic Potentials (MLIPs) enable molecular dynamics (MD) simulations with nearly quantum-chemical (QM) accuracy and have been successfully applied to various molecular systems. However, their systematic application to polymer systems has not yet been explored. A key challenge arises from the large molecular size, which makes QM reference calculations for the training data computationally demanding. Moreover, relaxation processes and diffusive behavior in polymers require long simulation times, making a direct comparison between MLIP-based and *ab initio* MD simulations infeasible.

In this study, we first train Atomic Cluster Expansion (ACE) potentials for small oligomers on MD reference data, thereby circumventing the need for expensive QM reference simulations and enabling long, cost-efficient MD trajectories. We then benchmark the transferability of the trained ACE potentials to longer polymer chains with respect to density, structural, and dynamic properties. The insights gained allow us to identify an optimal oligomer chain length that balances training cost and transferability. Based on this, we can efficiently train a QM-accurate potential for polymers on QM reference data in a second step.

CPP 46.54 Thu 9:30 P5

Fourth-Generation High-Dimensional Neural Network Potentials for Molecular Chemistry in Solution — •Djamil A. A. Maouene[1,2], Moritz R. 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 potentials have become essential tools in chemistry and materials science, offering accurate, efficient representations of high-dimensional potential energy surfaces for atomistic simulations. Here we compare two generations of high-dimensional neural network potentials (HDNNPs) 2G-HDNNPs and 4G-HDNNPs in their ability to model organic molecules in aqueous solution. 2G-HDNNPs perform well for systems dominated by local interactions because they rely on descriptors of the immediate atomic environment. However, in cases of long-range charge transfer 4G-HDNNPs provide a more reliable description by explicitly accounting for charge redistribution in the system as a function of its global structure. We illustrate these differences for organic molecules in water.

CPP 46.55 Thu 9:30 P5

Controlling porosity in supraparticles: A simulation study using spherical and rod-shaped particles — •Kritika Kritika[1,2], Mayukh Kundu[3], Michael Howard[3], and Arash Nikoubashman[1,2] — [1]Leibniz Institute of Polymer Research Dresden, Germany — [2]Institute of Theoretical Physics, TU Dresden, Germany — [3]Department of Chemical Engineering, Auburn University, Auburn, USA

Supraparticles (SPs) are large assemblies of smaller colloidal particles, whose properties can be tuned by modifying, e.g., the chemistry, shape, and size of the individual constituent particles and their arrangement within the SP. SPs can be formed through droplet drying, a process commonly observed in both everyday life and industrial applications, such as spray drying and printing. Porous SPs are of particular interest, since their high surface area and tunable pore size distribution make them ideal materials for catalysis, photonics, and adsorption applications. In this computational study, we explore the drying-induced formation of SPs made from spherical and rod-shaped particles. After drying, we selectively remove one of the particle components, leaving behind a highly porous SP. The initial volume fraction between spherical and rod-shaped particles plays a key role in shaping the porosity within the SP, while increasing the aspect ratio of the rods further amplifies the porosity of the SPs. Additionally, we observed that slower drying leads to a distinct increase in average pore size.

CPP 46.56 Thu 9:30 P5

Demystifying the decoupling of conformation and phase behavior in PNIPAM cononsolvency — •Ved Mahajan and Nico F. A. van der Vegt — Department of Chemistry, Technical University of Darmstadt

Cononsolvency describes the situation in which a polymer becomes insoluble in a mixture of two individually good solvents. PNIPAM, a widely studied thermoresponsive polymer, exhibits a strong coupling between its temperature-driven coil-globule transition and its phase behavior at low methanol concentrations; however, these two responses decouple as the methanol content increases. In this work, we use a minimal physical model, a hydrophobic polymer in water-methanol mixtures, that reproduces these key experimental observations. Despite its simplicity, the model captures both the emergence of cononsolvency and the crossover from coupled to decoupled thermal responses. At low methanol concentration, the polymer conformation remains temperature dependent, whereas at high methanol concentration, it becomes insensitive to temperature. In contrast, hydrophobic aggregation consistently strengthens with increasing temperature. Together, these results reveal a simple mechanism for the observed decoupling: the differing temperature sensitivities of polymer collapse and hydrophobic aggregation, both rooted in the hydrophobic effect.

CPP 46.57 Thu 9:30 P5

Molecular insights into the anion-dependence of the double-layer capacitance — •Richard Schömig[1], Xuqiang Xu[2], Jana Zaumseil[2], and Alexander Schlaich[1] — [1]Institute for Physics of Functional Materials, Hamburg Technical University, Hamburg — [2]Institute for Physical Chemistry, Heidelberg Universiy, Heidelberg

Mixed ionic-electronic conductors are promising candidates for organic electrochemical transistors (OECTs). Single-walled carbon nanotubes (SWCNTs), a key example, show transconductance and capacitance responses that are strongly influenced by the properties of the surrounding electrolyte [1]. To uncover the mechanisms governing this behavior, we perform molecular dynamics simulations of aqueous electrolytes containing ions of different sizes and concentrations under varying applied potentials. As a simplified model for the more complex SWCNT electronic structure, we here use graphene as the electrode material. Employing atomistic constant-potential simulations, we investigate how these electrolyte characteristics shape the interfacial structure and differential capacitance. Analysis of the hydrogen-bond network and associated free-energy changes highlights the central role of ion size in determining interfacial behavior.
[1] Xu, X.; Fresta, E.; Lindenthal, S.; Michel, E.; Zaumseil, J. ACS Appl. Mater. Interfaces 2025, 17(25), 37002-37011.

CPP 46.58 Thu 9:30 P5

Computing static and dynamic structure in colloidal models for solutions of globular proteins — •Sven Köbler — Institute of Applied Physics, University of Tübingen, Tübingen, Germany

Crowded solutions of globular proteins are commonly probed using neutron and X-ray scattering to obtain static and dynamic structure factors across a broad range of concentrations. Complementary insight can be gained from Brownian dynamics simulations based on coarse-grained colloidal models; however, extracting meaningful scattering observables particularly dynamic structure factors which requires fast and scalable trajectory analysis tools. We present an efficient computational framework for calculating both static structure factors $S(q)$ and intermediate scattering functions $F(q,t)$ directly from simulation trajectories. Our tools are highly optimized and build with CUDA compatibility to exploit computing speeds of GPUs. Its performance is demonstrated using binary colloidal models designed to mimic mixtures of bovine serum albumin (BSA) and ferritin. The resulting simulated scattering functions are compared with experimental X-ray photon correlation spectroscopy data.

CPP 46.59 Thu 9:30 P5

Dynamic properties of telechelic polyisobutylene with sticker ends: atomistic vs. coarse-grained molecular dynamics simulation — •Anastasiia Pivovarova and Viktor Ivanov — Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany

Modeling associating polymer networks, such as telechelic polyisobutylene (PIB) with barbiturate stickers, requires not only constructing accurate coarse-grained (CG) interaction potentials but also resolving the inherent problem of accelerated dynamics. This challenge becomes evident when comparing Green-Kubo viscosity calculations across different levels of resolution. Atomistic simulations of PIB with barbiturate end groups reproduce the expected rheological behavior of associating systems, yielding a viscosity of about 3.32 Pa*s. In contrast, CG simulations performed for pure PIB used as an initial step toward a full CG description of the telechelic system show a pronounced reduction in viscosity, reflecting substantially faster dynamics intrinsic to coarse-graining. These observations illustrate how dynamical acceleration can dominate the predicted viscoelastic properties even when structural features are reproduced, underscoring the need for systematic strategies to recover realistic dynamical behavior in CG models of associating polymer networks.

CPP 46.60 Thu 9:30 P5

Density of states in monodisperse and polydisperse hard disks: Concentration dependent SAMC estimation — •Viktor Ivanov, Joram Heimbold, Malte Kautzsch, and Timur Shakirov — Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany

We propose a new variant of flat-histogram Monte Carlo, where the density of particles is the control parameter for the density of states and the visiting histogram. We simulate a system of point particles with zero diameter. The square of the minimal interparticle distance, r^2_{min}, is used as the control parameter for a macrostate. The density of states and the visiting histogram depend on r^2_{min} and are updated at each step of the algorithm according to the usual SAMC rules. For a microstate (particilar configuration of particles) with a given value of the minimal distance between particles r_{min} one can replace the points with the hard disks of the diameter r_{min} or smaller, which corresponds to a system with a specific particle density. We apply this algorithm to 2d systems of monodisperse and polydisperse hard disks (with diameter distributions $1/d^2$) and study the density driven crystallization transition. For monodisperse hard disks the transition from the liquid to the hexatic phase proceeds via a first-order like pseudo-phase transition, whereas the transition from the hexatic to the crystalline phase is continuous. With increasing polydispersity, crystallization is significantly suppressed, such that no transition to the crystalline phase is observed for a 10% variation in particle radii.

CPP 46.61 Thu 9:30 P5

Benchmarking bond dissociation energies with plane-wave pseudopotential and Gaussian all-electron methods — •Yue Pan[1], Jochen Heil[2], Ali Karimi[2], and Arash Mostofi[1] — [1]Imperial College London, South Kensington Campus, London, SW7 2AZ, UK — [2]Continental Reifen Deutschland GmbH, Hanover, Germany

Accurate homolytic bond dissociation energies (BDE) are important for understanding bond breaking processes in molecules. They are also frequently used to benchmark the accuracy of different method for electronic-structure calculations. Most calculations of BDE focus on datasets of small gas-phase molecules and, accordingly, are carried out with localised-orbital methods, while systematic comparisons to periodic plane-wave DFT remain scarce. This is relevant for modelling interfacial failure processes in hybrid systems such as polymer nanocomposites, in which molecules are attached to inorganic surfaces, and it becomes less clear which method is more suitable from the perspective of accuracy and efficiency.

In this work, we benchmark the performance of two widely used approaches for DFT calculations, namely the plane-wave basis pseudopotential methods and Gaussian all-electron methods. We use C*C bond dissociation in gas phase hydrocarbons and surface-anchored molecules. We then compare our calculated BDEs with theoretical results obtained from highly accurate quantum chemistry methods and experimental values. Our work represents a step towards a better understanding of bond breaking and interfacial failure in materials.

CPP 46.62 Thu 9:30 P5

Continuum Modeling of Light-Matter Interaction in Polymer-Based Hollow-Core Optical Fibers with Different Geometrical Configurations — •Zehra Gizem Mutlay and Mustafa Ordu — UNAM - National Nanotechnology Research Center and Institute of Materials Science and Nanotechnology, Bilkent University, Ankara 06800, Türkiye

Recent studies have demonstrated that nested hollow-core optical fibers (HCFs) can achieve attenuation below 0.1 dB/km while maintaining broad transmission bandwidths. This performance demonstrates the promise of air-guided waveguides as alternatives to conventional solid-core optical fibers. In this work, we perform continuum modeling based on the finite-element method to investigate light interaction with polymer in HCFs by implementing three- and four-tube cladding structures. The analysis involves designs with and without nested elements and supporting bars. Our comparative investigation includes silica- and polymer-based structures to identify how intrinsic material properties and geometrical parameters influence mode confinement, optical loss, and transmission behavior. The findings show that even minor changes in geometry or material composition significantly influence light propagation, which underlines the sensitivity of optical guidance to light-material interaction. This study establishes a continuum-based framework for analyzing electromagnetic behavior in polymer systems and lays the groundwork for developing 3D-printed polymer-based hollow-core fibers with reduced attenuation for future applications in optical and materials physics.

CPP 46.63 Thu 9:30 P5

General Polarization Dependent Dynamic Light Scattering Using the Dynamic Mueller Matrix — •Reinhard Sigel — Independent Scientist, Markdorf, Germany

The Mueller Matrix for a general description of the polarization transfer of an optical system is combined with Dynamic Light Scattering (DLS) [1]. Azzam's procedure [2] based on two rotated quarter wave plates is combined with photo correlation measurements to detect the Dynamic Mueller Matrix, which contains all possible polarization dependent correlation functions. The related Siegert relation is derived. Applications are dynamic ellipsometric light scattering [3] experiments on soft colloidal particles and 3D correlation ellipsometry [4] experiments on soft interfaces [5].

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CPP 46.64 Thu 9:30 P5

Versatile X-Ray Reflector Extension Setup for Grazing-Incidence Experiments for Liquid Surface Study at the Beamline P03/PETRA III — •Jan Rubeck, Andrei Chumakov, and Matthias Schwartzkopf — DESY, Notkestr. 85, 22607 Hamburg, Germany

Existing beamlines for in situ GISAXS on liquids are either limited in angular range or incompatible with the large sample-detector distance required for submicron resolution. We present a low-cost, easily assembled beam-tilting extension for synchrotron-based ultra-small-angle X-ray scattering (USAXS) facilities, enabling grazing-incidence (GI-) and transmitted scattering (GIUSAXS, GTUSAXS) studies on liquid surfaces. The setup is compatible with standard USAXS beamlines and requires only 0.5 m of space at the sample stage. It allows X-ray beam incidence angles of up to 0.6° at the liquid surface, equal to twice the angle of incidence on a reflector and below its critical angle of reflector materials, and provides access to a q-range of approximately 0.003-0.5 nm^{-1}. The system was tested at P03 beamline (DESY) using polystyrene nanoparticles, self-assembled at the air/water interface. The proposed scheme enables selective depth profiling and expands the research capabilities of existing SAXS synchrotron facilities for in situ studying submicron nanostructured objects at liquid surfaces under GI-geometry, combined also with GIWAXS and TXRF techniques. https://doi.org/10.1107/S1600577525003431

CPP 46.65 Thu 9:30 P5

Hybrid field coupling in nanoscale infrared spectroscopic imaging of nano-structured soft matter — •Sharon Xavi[1], Mashiat Huq[1], Matthias Zeissberger[2], Daniela Täuber[1,2], and Christin David[1,3] — [1]Friedrich Schiller University Jena, 07743 Jena — [2]Leibniz Institute of Photonic Technology, 07745 Jena — [3]University of Applied Sciences, 84036 Landshut, Germany

Anisotropic intensity distributions are frequently observed on nanostructured surfaces in the emerging field of nanoscale infrared (IR) spectroscopic imaging methods, including mid-IR scattering scanning optical nearfield microscopy (IR-sSNOM) and methods combining mid-IR illumination with mechanical detection using atomic force microscopy (AFM-IR). Such methods bridge the gap between high-resolution structural imaging in electron and atomic force microscopy and chemical imaging in conventional far-field IR spectroscopy by overcoming the limitations of optical diffraction in far-field IR spectroscopic imaging. In the mid-IR spectral region, the hybrid field coupling of the incident field with a polymer nanosphere and a metallic AFM probe is nearly as strong as the plasmonic coupling in case of a gold nanosphere [Anindo et al., J. Phys. Chem. C, 2025, 129, 4517]. We modeled this hybrid field coupling on varied nanostructured surfaces to enhance the understanding of the observed anisotropies and contribute to the development of advanced applications of these methods [Ali et al. Anal. Chem., 2025, 97, 23914].

CPP 46.66 Thu 9:30 P5

Learn how to switch off: In-silico Modelling of Thermal Ring-closing Process in Spiropyran Derivatives — •Bowen Cheng, Robert Strothmann, Hendrik Heenen, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin, Germany

Spiropyran (SP) and its derivatives undergo a ring-opening reaction via UV radiation and a ring-closing reaction in thermal conditions, making them excellent candidates for photoswitches. One key aspect that governs the sensitivity of such photoswitches is the rate of the thermal ring-closing process. A main challenge in modelling this process is the existence of various thermally accessible conformers, leading to a complex reaction network.

In this study, we highlight a combined workflow using machine-learned interatomic potential (MLIP) and a microkinetics model (MKM) to address this. With a fine-tuned MACE-OFF24 foundation model, we predict different transition state energies within the reaction network using the nudge elastic band method, and correlate these energies to experimental observations using the MKM.

Our workflow can be migrated between different SP derivatives to reveal the effect of functional group decorations. Our findings demonstrate the potential of using MLIPs to predict transition states and enable larger-scale studies of complex reaction networks. We also aim to condense our workflow as a new descriptor for *in-silico* screening in future spiropyran photoswitch design.

CPP 47: Focus Session: Controlling Microparticles and Biological Cells by Ultrasound (joint session BP/CPP/DY)

Recently ultrasound has emerged as a very promising physical modality to control the behavior of microparticles and even of biological cells, which can be moved and stimulated by sound waves. For biological cells, one can further control the effect of sound through gene expression (sonogenetics), similar to the control by light (optogenetics). However, because the wavelength of sound is much larger than the one of light, one of the challenges is to localize the effect of sound waves, e.g. by using gas bubbles. Here, we bring together experimental and theoretical researchers who currently explore the potential of ultrasound to control active and passive microsystems and to develop new applications ranging from biomedicine to soft robotics.

Organized by Peer Fischer and Ulrich S. Schwarz (Heidelberg)

Time: Thursday 10:15–12:45 Location: BAR/0106

Invited Talk CPP 47.1 Thu 10:15 BAR/0106

Mechanogenetics for Cell ImmunoTherapy — •Yingxiao Wang — 1002 childs way, Los Angeles, CA 90089

Cell-based cancer immunotherapy is a promising therapeutic intervention for cancer treatment. However, non-specific toxicity against healthy tissues (e.g. off-tumor toxicity) is a major hurdle for solid tumor treatment. We have developed controllable on-switch gene cassettes in which a specific antigen production on the target cancer cell can be remotely and mechanically induced by an external focused ultrasound (FUS). FUS was applied to stimulate the production of the synthetic and clinically validated antigen on tumor cell surface orthogonal to the endogenous proteins. SynNotch was further engineered into primary human T cells (SynNotch-CAR T) to recognize the synthetic antigen expressed on the ultrasound-induced tumor cells and activate the production of CAR, which can lead to the recognition of a native tumor specific antigen (TSA) universally expressed on the whole population of tumor cells for immunotherapy. We applied this system to treat prostate cancer cells whose locally metastasized tumors are confined in space but intermingled with vessels and nerves. Our results showed that FUS can mechanically induce the synthetic antigen production in prostate cancer cells, which results in the engagement and activation of SynNotch CAR T cells for the tumor eradication. This local activation of engineered tumor cells by FUS should allow a high precision and safety in eradicating tumors. Hence, this approach for immunotherapy should open new opportunities to integrate engineering mechanics with genetic medicine for successful translation.

CPP 47.2 Thu 10:45 BAR/0106

Shaping sound to tickle cells — •Dimitris Missirlis[1,2], Athanasios Athanassiadis[1,2], Rom Lerner[1,2], and Peer Fischer[1,2] — [1]Institute for Molecular Systems Engineering and Advanced Materials, Im Neuenheimer Feld 225, 69120 Heidelberg, Germany — [2]Max Planck Institute for Medical Research, Jahnstr. 29, 69120, Heidelberg, Germany

The ability to shape ultrasonic waves precisely is finding growing relevance in biomedical applications, where ultrasound is increasingly used to noninvasively stimulate biological tissues for therapeutic purposes. However, it remains an unsolved question how high-frequency ultrasound can interact with cells to excite biological responses. Our recent work on shaping and controlling ultrasound waves has provided us with a new tool to address the fundamental question how ultrasound interacts with and influences cells. To this end we have developed adaptable setups where we can control relevant ultrasound parameters in vitro as well as in vivo. By systematically examining the critical parameters, we discuss the role of different ultrasonic effects, including thermal effects, radiation forces, and sound-induced shear flows. Further, we discuss both physical and sonogenetic methods that can be used to enhance the coupling of ultrasound to cells.

CPP 47.3 Thu 11:00 BAR/0106

A Theoretical Model for Ultrasound-Induced Intracellular Streaming — •Niels Gieseler[1,2,3], Falko Ziebert[1,2], and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, Heidelberg 69120 Germany — [2]BioQuant, Heidelberg University, im Neuenheimer Feld 267, Heidelberg 69120 Germany — [3]Max Planck Institute for Medical Research, Jahnstrasse 29, Heidelberg 69120, Germany

Ultrasound is not only the basis of an essential imaging method for biomedicine, recently it has also become a promising avenue to control biological systems, for example, in sonogenetics or ultrasound neuromodulation. However, the underlying physical effects are not well understood, and a complete theoretical description is missing. In fact, many different physical effects compete, including radiation forces, streaming, cavitation, and local heating. Here, we focus on intracellular streaming, which might induce organelle movement or alter gene expression, as the steady second-order rotational flow generated by an acoustic source. As a model for the viscoelastic nature of cells and their surroundings, we use Oldroyd-B fluids. Building on existing work, we calculate the streaming flows inside and outside of a sphere sonicated with a plane wave. The streaming is treated as a second-order perturbation expansion of the Navier-Stokes equations, which is solved separately for both media and combined using suitable boundary conditions. Our work shows under which conditions intracellular streaming can be induced in biological cells.

15 min. break

Invited Talk CPP 47.4 Thu 11:30 BAR/0106

Recent theoretical progress on sound-propelled microsystems — •Raphael Wittkowski — Department of Physics, RWTH Aachen University, 52074 Aachen, Germany — DWI – Leibniz Institute for Interactive Materials, 52074 Aachen, Germany

The research area of sound-propelled microsystems is growing fast and has a great potential for various future applications in engineering, medicine, and other fields. The progress in this area is accelerated by theoretical methods, as analytical modeling and computer simulations can provide new insights that cannot be obtained by experiments.

In this talk, I will address the theoretical investigation of sound-propelled microsystems and present examples from the recent research progress in this area. The talk will cover different types of sound-propelled microsystems including microrobots, micromachines, artificial muscles, and soft robots.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – 535275785.

CPP 47.5 Thu 12:00 BAR/0106

Rarefaction wave amplification from non-resonant deforming bubbles — Yuzhe Fan, Saber Izak Ghasemian, and •Claus-Dieter Ohl — Otto-von-Guericke University, Magdeburg, Germany

Gas bubbles in liquids or soft matter exposed to acoustic waves behave as oscillators, with maximum response at their resonance frequency. When driven below resonance at sufficient pressure amplitudes, bubbles can collapse with strong energy focusing and even emit light; when driven near resonance, surface instabilities and fast jet flow develop during oscillation. Like other oscillators, bubbles cease to respond when driven far above resonance. Although their oscillations are minimal, bubbles in this regime act as pressure-release interfaces, can reflect high peak pressure shock into rarefaction wave, and may therefore seed cavitation when interacting with high-power therapeutic ultrasound. Yet, here we show that even diagnostic ultrasound with peak positive pressures as low as $\sim$10 MPa can nucleate cavitation in microseconds. This is caused through the non-resonant deformation of the bubble into a concave shape that refocuses scattered waves, amplifying the tension leading to microcavitation. Our findings reveal that cavitation can be triggered by high-frequency positive pressure over a much wider amplitude range than previously recognized, offering a new perspective for current safety guidelines for ultrasound bioeffects and applications in medical ultrasound.

CPP 47.6 Thu 12:15 BAR/0106

Optimizing acoustically propelled microrobots using genetic algorithms — •Lennart Gevers[1,2,3] and Raphael Wittkowski[1,2,3] — [1]Department of Physics, RWTH Aachen University, Aachen, Germany — [2]DWI – Leibniz Institute for Interactive Materials, Aachen, Germany — [3]Institute of Theoretical Physics, Center for Soft Nanoscience, University of Münster, Münster, Germany

The promising potential applications of acoustically propelled microparticles demand methods to create particle designs that allow for targeted autonomous motion. Current methods remain largely based on experiments due to the intricate nature of the underlying dynamics. Large-scale computational studies, specifically when combined with optimization algorithms, are impeded by the cost of traditional acoustofluidic simulations.

In this talk, we present the implementation of an analytical framework describing non-Brownian motion of colloidal molecules driven by acoustic streaming. The analytical framework is combined with vectorized, GPU-accelerated, and distributed computation. This enables fast, large-scale simulations, where 10^5 trajectories over 10 s real time can be simulated on a normal personal computer within one minute. Coupling this approach with genetic algorithms reveals particle geometries, control parameters, and underlying principles for acoustically propelled particles that exhibit controllable and stable behavior over long times.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – 535275785.

CPP 47.7 Thu 12:30 BAR/0106

Equations of motion for arbitrarily shaped acoustically propelled rigid microparticles — •Justus Schnermann[1,2,3] and Raphael Wittkowski[1,2,3] — [1]Department of Physics, RWTH Aachen University, Aachen, Germany — [2]DWI – Leibniz Institute for Interactive Materials, Aachen, Germany — [3]Institute of Theoretical Physics, Center for Soft Nanoscience, University of Münster, Münster, Germany

Much experimental research concerns the acoustic propulsion of microparticles, but theoretically, only axisymmetric particles with a stable orientation have been studied thus far. In this talk, we present an analytical derivation of the ordinary differential equation of motion for an arbitrarily shaped acoustically propelled rigid microparticle. This equation governs the time evolution of the orientation and position of the particle. Its parameters depend only on the particle's leading-order oscillation velocity field. Based on this equation, we classify qualitatively the possible long-term trajectories of arbitrary particles in unidirectional ultrasound.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – 535275785.

CPP 48: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VI

Time: Thursday 11:30–12:45 Location: ZEU/LICH

CPP 48.1 Thu 11:30 ZEU/LICH

Simulating Light Induced Phase Separation in Mixed Halide Perovskites — •Sebastian Schwartzkopff, Ivan Zaluzhnyy, Ekatarina Kneschaurek, Paul Zimmermann, Dmitry Lapkin, Hans Mauser, Alexander Hinderhofer, and Frank Schreiber — University of Tübingen

By varying the halide composition in mixed organic-inorganic perovskites such as MAPbBr$_{1.8}$I$_{1.2}$ (MA-methylammonium), one can precisely tune the band gap. This is a desirable property for solar cell design, as it allows for the production of high efficiency solar cells. However, illumination with visible light drives these materials to phase-separate into Br-rich and I-rich domains, thereby degrading the tuned bandgap. To better understand and potentially control this behavior, we employ phenomenological approaches such as Cahn-Hilliard and Monte Carlo models. While Cahn-Hilliard methods were initially explored, they proved challenging in reproducing experimentally observed dynamics. On the other hand, Monte Carlo methods have shown themselves to enable a systematic exploration of how factors such as halide ratio, charge-carrier density, temperature, and illumination intensity influence light-induced phase separation. Overall, we found that Monte Carlo simulations, with appropriately chosen parameters, can successfully reproduce key features observed in experimental diffraction measurements.

CPP 48.2 Thu 11:45 ZEU/LICH

Reorientation-driven degradation in oriented perovskite films: shifting facet engineering to thermodynamic stability — •Xiaojing Ci[1], Xiongzhuo Jiang[1], Guangjiu Pan[1], Kun Sun[1], Altantulga Buyan-Arivjikh[1], Zerui Li[1], Lixing Li[1], Thomas Baier[1], Matthias Schwartzkopf[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]DESY, Hamburg

Hybrid perovskite solar cells suffer from underexplored links between crystallographic orientation and thermal stability. We fabricate highly oriented mixed Sn-Pb perovskite films via an additive-free two-step method. Accelerated aging studies under high temperature reveal that high orientation paradoxically compromises stability and PSCs built from highly oriented perovskite films retain only 73% of their initial PCE versus 89% in less-oriented devices. Operando GIWAXS of the PSCs shows that thermal stress induces significant reorientation and lattice distortion in the oriented crystallites. Structural analyses confirm progressive crystallographic transitions, including grain reconfiguration, shifts toward isotropy, and systematic diffraction migrations. Critically, we demonstrate that metastability is an intrinsic consequence of high crystallographic order, which is why the very high alignment strategies that enhance performance induce thermodynamic vulnerability. This necessitates redesigning crystal engineering priorities where suppressing instability requires engineering thermodynamic equilibrium states over maximizing alignment for stable perovskite photovoltaics.

CPP 48.3 Thu 12:00 ZEU/LICH

Understanding the molecular origins of giant surface potential: a case study of TPBi — •Mauricio Sevilla[1], Naomi Kinaret[1], Muhammad Nawaz Qaisrani[1,2], Albin Cakaj[4], Alexander Hofmann[4], Falk May[3], Wolfgang Brütting[1], and Denis Andrienko[4] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Technische Universität Ilmenau, Ilmenau, Germany — [3]Merck Electronics KGaA, Darmstadt, Germany — [4]University of Augsburg, Augsburg, Germany

In the context of organic light-emitting diodes, the molecular orientation in thin layers of organic materials plays a crucial role in charge injection, light outcoupling, and the formation of internal electrostatic fields due to the alignment of molecular dipoles. This latter phenomenon is referred to as the giant surface potential (GSP). Predicting GSP soleley from the chemical structure is challenging, as it is highly sensitive to processing conditions such as temperature and deposition rate during the physical vapor deposition process. Using both all-atom and coarse-grained simulations, we develop and test a framework capable of predicting the molecular ordering of organic materials under varying substrate temperatures and deposition rates. The framework's accuracy is validated by comparing the predicted GSP and birefringence of thin films to experimentally measured values, for a series of TPBi isomers.

CPP 48.4 Thu 12:15 ZEU/LICH

Additives to enhance efficiency and stability of PPDT2FBT:PC60BM organic solar cells — •Hassan Ismail[1,2], Jose Prince Madalaimuthu[1,2], Ulrich Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstrasse 10, 07743 Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

The development of organic solar cells (OSCs) requires simultaneous optimization of photovoltaic performance and long-term thermal stability, often mediated by processing solvents and additives. This study investigates the role of small amphiphilic molecules (AMs) as surfactants in stabilizing the bulk heterojunction morphology of PPDT2FBT:PCBM-based OSCs. Our research goal is to understand how the chemical nature of AMs and their interface engineering within the device affect stability and efficiency. We demonstrate that the AM's polar headgroup chemistry is a critical determinant for operational stability, and by strategically applying interface engineering across all major interfaces, we identify optimal scenarios for enhancing both efficiency and device durability. Interface engineering not only improves charge transport and mitigates degradation but also supports large-area fabrication and practical device reliability, addressing prominent challenges for commercialization. These findings guide future molecular design and interface engineering strategies, contributing to the realization of more robust and reliable organic solar cells.

CPP 48.5 Thu 12:30 ZEU/LICH

Controlling singlet fission in diketopyrrolopyrole diner through solvent choices — •Sruthy Asa Rajan[1,2], Isaac M. Etchells[3], Jegadesan Subbiah[2], Sergey Bagnich[1], Paul E. Shaw[3], David Jones[2], and Anna Köhler[1] — [1]Universität Bayreuth — [2]University of Melbourne — [3]University of queensland

The efficiency of conventional solar cells is constrained by the Shockley-Queisser limit, which is arises from thermalisation loss. Singlet fission (SF) 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 separation. PDPP is a molecule with a comparable triplet energy to the silicon bandgap. But monomer molecules are not SF active in solution. We prepared PDPP-dimers with a pyrene bridge. We investigate the influence of solvent properties on the optical behaviour of these N-alkylated pyrene-bridged PDPPs. We employ temperature-dependent steady-state and time-resolved photoluminescence studies on N-alkylated pyrene-bridged PDPPs in protic polar and aprotic polar solvents to study the optical properties of the evolution of different species. At an intermediate temperature, we observed an intermediate emission, which then, on further decreasing the temperature (less than 100K), is replaced by 1(TT) emission. We also measured TA on different solvents which showed different pathway. In protic polar solvent, our molecule showed intermolecular SF whereas in aprotic polar solvent it showed intermolecular

CPP 49: Gels, Polymer Networks and Elastomers I

Time: Thursday 11:30–12:45 Location: ZEU/0255

CPP 49.1 Thu 11:30 ZEU/0255

Nanoparticle–Polymer Coupling in Magnetic Gels Studied by Means of Computer Simulations and Experiments — •Rebecca Stephan[1], Surojit Ranoo[2,4], Patrick Kreissl[1], Chinmay Pabshettiwar[1], Jessica Kubis[2], Christian Holm[1], Annette M. Schmidt[2], Regine von Klitzing[3], and Rudolf Weeber[1] — [1]Institute for Computational Physics (ICP), Universität Stuttgart — [2]Institute of Physical Chemistry, Department of Chemistry, University of Cologne — [3]Institute for Condensed Matter Physics, Technical University of Darmstadt — [4]Laboratoire Colloïdes et Matériaux Divisés, ESPCI Paris

Magnetic gels - soft hydrogels with embedded magnetic nanoparticles (MNPs) - combine the viscoelastic properties of a gel with the magnetic behavior of the MNPs. Their response to an external magnetic field enables tunable mechanical and dynamic properties such as shape, stiffness, and swelling. The microscopic coupling mechanisms between the MNPs and the surrounding polymer matrix are crucial for the material's stimuli-responsive properties. However, these mechanisms are not yet fully understood.

In this work, we juxtapose results for PAAm hydrogels with embedded cobalt ferrite nanoparticles with coarse-grained molecular dynamics simulations coupled to lattice-Boltzmann hydrodynamics. In both cases, we probe the coupling using magnetic AC susceptibility spectra. Our findings demonstrate that the local polymer environment and the surface heterogeneity of the magnetic particles - chemical or topographical - play an important role in MNP-polymer coupling.

CPP 49.2 Thu 11:45 ZEU/0255

Strain-stiffening critical exponents of fibre networks under uni-axial deformation — •Atharva Pandit[1] and Abhinav Sharma[1,2] — [1]Institut für Physik, Universität Augsburg, 86159 Augsburg, Deutschland — [2]Bereich Theorie der Polymere, Leibniz-Institut für Polymerforschung, 01069 Dresden, Deutschland

Disordered fibre networks exhibit a floppy to rigid mechanical phase transition as a function of connectivity. Sub-isostatically connected networks can undergo this transition via straining. Critical exponents governing this transition have been estimated theoretically and by numerical simulations of various types of networks. We present improved results, achieved through a combination of refined numerical simulations, larger system sizes and incorporation of theoretical predictions for better post-simulation analysis. A linear evolution of the critical strain and critical exponents is observed as the network is sheared while being subjected to non-volume-preserving uni-axial deformations.

CPP 49.3 Thu 12:00 ZEU/0255

Probing Mechanical Properties of Magnetic Gels Using Computer Simulations — •Yashas Tejaskumar Gandhi, Christian Holm, and Rudolf Weeber — Institute For Computational Physics, University of Stuttgart, Germany

Magnetic gels are liquid swollen polymer networks embedded with magnetic nanoparticles (MNPs). Their motion, shape and mechanical properties can be governed by an external magnetic field. The mechanical properties of a magnetic gel depend on both the polymer network and the embedded MNPs. They can also be heated by applying an AC magnetic field due to viscous and hysteresis losses.

There are two ways to probe the mechanical properties of magnetic gels: at the nanoscopic level using AC susceptometry, and at the macroscopic level by measuring stress under deformation. While macroscopic measurements are relatively straightforward, they are computationally demanding. The Gemant-DiMarzio-Bishop theory provides a framework for connecting magnetic AC susceptibility data to nanoscale mechanical properties. Our objective is to test this theory in computer simulations by comparing nanoscale measurements with macroscale measurements.

The polymer network is modelled as a coarse-grained bead-spring system. We also incorporate a solvent model for hydrodynamic interactions in the system. Shear deformation is applied using periodic Lees-Edwards boundary conditions. Our simulations use the 'Extensible Simulation Package for Research on Soft Matter Systems (ESPResSo)' simulation package.

CPP 49.4 Thu 12:15 ZEU/0255

Dynamic control of rigidity via geometric frustration — •Santiago Gomez Melo[1,2], Falko Ziebert[1,2], and Ulrich S. Schwarz[1,2] — [1]ITP, Philosophenweg 19, Heidelberg — [2]BioQuant, Im Neuenheimer Feld 267, Heidelberg

Recent advances in materials design and 4D-printing now allow one to realize programmable metamaterials that upon receiving a suitable stimulus dynamically change their unconventional macroscopic properties. For mechanical metamaterial, these tunable features have so far been restricted to geometric quantities, such as the Poisson ratio and the strain-to-twist ratio, but the effective elastic moduli have not been addressed yet. Here we combine central force network theory and responsive hyperelasticity to show that it is also possible to dynamically control the elastic moduli, and more specifically the shear modulus, by programming geometric frustration into a stimuli-responsive structure. This phenomenon, known as geometric incompatibility, produces a rigidity phase transition in which the elastic modulus changes by several orders of magnitude. It results from inducing a state of self-stress that eliminates the floppy modes of the system by producing second-order rigidity. The underlying physical principle seems to be also at work in biological systems, most prominently in epithelial monolayers, but here it is predicted for entirely synthetic materials, like temperature-sensitive hydrogels and nematic elastomers, opening up the perspective of designing a new class of dynamic metamaterials.

CPP 49.5 Thu 12:30 ZEU/0255

Aqueous Foams stabilized by PNIPAM Microgels: Effect of Cross-linker and Concentration — •Joanne Zimmer, Kevin Gräff, Luca Mirau, and Regine von Klitzing — Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 8, D-64289 Darmstadt

Aqueous foams are abundant in everyday life, important for industrial applications and interesting from a fundamental point of view. In this work, aqueous foams are generated by sparging gas (nitrogen) through an aqueous dispersion of PNIPAM microgels, which are used as foam stabilizers. The microgel cross-linker content as well as the microgel concentration are varied and prove to significantly influence the foam formation properties (foamability) and the foam stability. A lower cross-linker content as well as a higher microgel concentration elevate the foamability, generate foams with higher liquid content and smaller bubbles and increase the foam stability. These observations are correlated with the microgel behaviour at the single air-water interface, i.e. pendant drop measurements and Langmuir trough. Our findings highlight good agreement across both length scales: an increase in foamability correlates with a faster decrease in surface tension, and a higher foam stability with a higher surface elastic modulus of a microgel-covered single air-water interface. The ability of the microgels to form a collective polymer network seems to dominate these processes.

CPP 50: Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates II (joint session CPP/BP)

Time: Thursday 11:30–12:45 Location: ZEU/0260

CPP 50.1 Thu 11:30 ZEU/0260

Exponential Size Control in Biomolecular Condensates via Universal Scaling of Power-Law Distributions — •Yifan Huang[1], Chuan Tang[1], Haoyu Song[2], Bing Miao[3], and Qiyun Tang[1,4] — [1]Key Laboratory of Quantum Materials and Devices of Ministry of Education, School of Physics, Southeast University, Nanjng 211189, China — [2]School of Physics, Zhejiang University, Hangzhou 310058, China — [3]Center of Materials Science and Optoelectronics Engineering, College of Materials Science and Opto-Electronic Technology, University of Chinese Academy of Sciences, Beijing 100049, China — [4]Jiangsu Physical Science Research Center, Nanjing 210093, China

Power-law distributions are ubiquitous phenomena in diverse systems, whereas concomitant scale invariance hinders the exploration of precise size control for biocondensates in recent experiments. Using massive computer simulations and the kinetic theory of coalescence, we demonstrate that the cutoff volume can collapse all power-law distributions of biocondensates in different parameters onto one master curve. Remarkably, the cutoff size can increase exponentially by increasing monomer concentrations $R \sim e^{\phi}$, of which nanometer condensates in simulations can be extrapolated to micrometer droplets in experiments. The findings provide a new mechanism to rapidly tailor the biocondensates to appropriate sizes through power-law distributions, which can stimulate explorations in biological and other nonequilibrium systems

CPP 50.2 Thu 11:45 ZEU/0260

Droplet-assisted folding of long regulatory RNAs — Simon Doll[1], Lukas Pekarek[1], Fathima Ferosh[1], Jovana Vasiljević[1], Marcus Jahnel[1], and •Tyler Harmon[2] — [1]BIOTEC, Dresden, Germany — [2]IPF, Dresden Germany

Long regulatory RNA regions orchestrate complex cellular processes, including gene expression and epigenetic modifications. How these RNAs dynamically fold and refold in response to cellular signals remains poorly understood. Given that RNAs interact with ubiquitous RNA-binding proteins (RBPs) prone to form biomolecular condensates, we explore how protein droplets interacting along an RNA impact its folding process. Attached droplets prevent premature folding by competing with RNA:RNA interactions. When droplets dissolve due to cellular signals, capillary effects cause the RNA to collapse while refolding. We test this process of condensate-guided RNA folding by adapting established RNA secondary structure predictors to mimic various folding pathways and supplement this with coarse-grained simulations. We find that interactions with transient droplets robustly leads to the formation of long-range RNA contacts, which are otherwise hard to achieve. Our results compare favorably with available experimental data. We propose that this strategy, which we call droplet-assisted RNA folding, represents a previously unexplored mechanism for shaping RNA structures. Given the widespread propensity of RBPs to form condensates, this process could play a fundamental role in the structural organization, conditional reshaping, and functional regulation of long regulatory RNAs.

CPP 50.3 Thu 12:00 ZEU/0260

Simulation Insights into the Assembly of Polyplexes for RNA Delivery — •Jonas Hans Lehnen[1], Jorge Moreno Herrero[3], Heinrich Haas[3], Friederike Schmid[1], and Giovanni Settanni[1,2] — [1]Department of Physics, Johannes-Gutenberg University Mainz — [2]Faculty of Physics and Astronomy, Ruhr University Bochum — [3]BioNTech SE, Mainz

RNA-based pharmaceuticals proved successful with the COVID-19 vaccines and are now undergoing clinical trials for a broad range of therapeutic indications. Lipid-based nanoparticles (LNPs) have been used so far as delivery systems, although alternatives are still needed to meet efficacy and safety requirements across a broader range of applications. Polyplexes, formed by the self-assembly of cationic polymers with the anionic nucleic acids, constitute a valuable substitute, especially if precise control of the number and shape of the encapsulated RNA chains is possible. Here[1], we use molecular dynamics simulations of a coarse-grained polyplex model to show that the most important factors controlling it are the charge ratio between polyelectrolytes and RNA and their concentration during assembly. Close to the isoelectric point, the polyplexes are large, whereas in large excess of cationic polymer, their size decreases, allowing one RNA copy per nanoparticle. Our results are consistent with recent experimental work on polyethylenimine polyplexes.

[1] Simulation Insights into the Assembly of Polyplexes for RNA Delivery, Lehnen et al., Biomacromolecules (2025), DOI: 10.1021/acs.biomac.5c01219

CPP 50.4 Thu 12:15 ZEU/0260

Polymer-assisted condensation as key to chromatin localization — •Arghya Majee[1] and Jens-Uwe Sommer[1,2,3] — [1]Leibniz Institute of Polymer Research Dresden, Germany — [2]Institute for Theoretical Physics, TU Dresden, Germany — [3]Cluster of Excellence Physics of Life, TU Dresden, Germany

We put forward a novel mechanism [1] to account for the experimentally observed [2] positional shifts of chromosomes within the cell nucleus, which appear to be driven by compositional alterations in the nuclear lamina. By considering chromatin as a biomolecular condensate we demonstrate that the adsorption of the chromatin-binding proteins at the lamina leads to a wetting of the condensate while spreading of the chromatin on the lamina is avoided. This leads to the nonmonotonous density profile of the polymer with respect to the surface which can be explained by the competition between the tendency of the protein component to wet the surface and the conformational restrictions of the polymer near the impenetrable surface. A change in the composition of the the lamina can lead to repositioning of chromatin towards the center of the nucleus. Our theory not only offers an explanation for specific chromatin conformation experiments, but also contributes to the broader understanding of wetting onto responsive surfaces in multi-component systems.

References:

[1] A. Majee and J.-U. Sommer, bioRxiv 2025.06.11.658974 (submitted).

[2] Amiad-Pavlov *et al.*, Sci. Adv. **7**, eabf6251 (2021).

CPP 50.5 Thu 12:30 ZEU/0260

Bridging Scales to Understand the Role of Ubiquitylation and Sumoylation in Protein Phase Separation — •Supriyo Naskar, Kurt Kremer, and Oleksandra Kukharenko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

The post-translational modifiers, such as mono- and poly-ubiquitins and SUMOs, are known for their ability to modulate protein-protein interactions by becoming covalently attached to other target proteins. Despite the high similarity in the tertiary structure and sequence, they differentially influence the target protein properties. In this work, we employed a multiscale simulation approach that encompasses atomistic to different levels of coarse-grained modeling techniques, combined with data-driven methods, to explore the structural differences and multidimensional energy landscapes of ubiquitin, SUMO, and their conjugates. We finally investigate the influence of distinct features of the targets and modifiers on protein phase separation and aggregation, providing molecular-level insight into the corresponding in vitro measurements and informing further experiments through the adjustment of relevant parameters.

CPP 51: Focus Session: 75 Years Polymer Physics Division: From Curiosity to Smart Materials (joint session CPP/BP)

Polymer materials are ubiquitous in modern society. In recent years, the focus has been on the development of functional, tunable or responsive materials, oftentimes inspired by biological materials. At this, a number of fundamental problems arise, e.g. regarding the interaction of polymers with water, biomolecules or inorganic nanoparticles and the resulting self-assembled morphologies as well as the underlying dynamics and the kinetics of morphological changes upon a stimulus. These problems are nowadays addressed in an interdisciplinary way by experimental methods, computer simulations and theory, often in close collaboration with polymer chemists. In five talks by renowned speakers, the focus session aims at highlighting few of these aspects that are currently under investigation worldwide. The fact that the Polymer Physics Division of the German Physical Society was founded in 1951 and hence, 2026 is the 75th anniversary, seems to be a good occasion to bring modern polymer physics into the focus.

Organized by Christine M. Papadakis, Christian Holm, Tayebeh Ameri and Kristian Franze.

Time: Thursday 15:15–17:45 Location: ZEU/LICH

Topical Talk CPP 51.1 Thu 15:15 ZEU/LICH
The Loops of Life — Brian Chan and •Michael Rubinstein — Duke University, Durham, NC, USA

In mammalian cells, the cohesin protein complex is believed to regulate chromatin during interphase through active loop extrusion, in which dynamic loops are formed by cohesin translocating along chromatin. We developed a theoretical model that quantifies how key parameters, including cohesin residence time on chromatin, extrusion velocity, and the number density of chromatin-bound cohesins, regulate genomic contacts. The model describes chromatin contact probabilities and predicts that loop formation probability is a nonmonotonic function of loop length. Our theory demonstrates that active loop extrusion causes the apparent fractal dimension of chromatin to cross over between two and four at contour lengths on the order of 30 kilobase pairs. This work provides a theoretical basis for the compact organization of interphase chromatin, explaining the physical reason for the segregation of topologically associated domains and suppression of chromatin entanglements by up to a factor of 50, which contributes to efficient gene regulation by distal elements such as enhancers or silencers.

Topical Talk CPP 51.2 Thu 15:45 ZEU/LICH
Polyelectrolytes and Biological Systems: A Charged Relationship — •Matthias Ballauff — Chemie und Biochemie, Freie Universitaet Berlin

If charges are appended to linear or crosslinked polymers, a polyelectrolyte results. Polyelectrolytes are ubiquitous and play a major role in biophysics. Important natural polyelectrolytes as e.g. DNA or Heparin are central in biology, and a thorough understanding of these systems and of charge-charge interaction is one of the main tasks of biophysics. In my lecture, I will discuss our recent research done on -Interaction of linear polyelectrolytes with proteins. This problem is also relevant for the formation of biocondensates by the interaction of cationic and anionic proteins; -Charged polymer networks and their interaction with proteins; -Role of polyelectrolytes in virus infections. In all cases, a quantitative understanding of the systems in terms of analytical models can be achieved, which may pave the way for future pharmaceutical applications.

Topical Talk CPP 51.3 Thu 16:15 ZEU/LICH
From block copolymer morphologies to functional polymer membranes — •Volker Abetz — Helmholtz-Zentrum Hereon, Institute of Membrane Research, Max-Planck-Str. 1, 21502 Geesthacht, Germany — University of Hamburg, Institute of Physical Chemistry, Martin-Luther-King-Platz 6, 20146 Hamburg, Germany

Depending on solvent selectivity and the time of evaporation different structures can be obtained in cast block copolymers, showing that there is an interplay between kinetics and thermodynamic driving forces during the self-assembly before the sample is dry. When preparing membranes from block copolymer solutions, besides molecular weight, composition of the block copolymer and its concentration, also the choice of solvent, and the casting conditions play an important influence on the obtained morphology of the finally obtained membrane. This is especially important when membranes are prepared via the so-called non-solvent induced phase separation process after initial self-assembly by partial evaporation of solvent. The obtained membranes, when prepared successfully, display a rather isoporous top layer and can be subsequently post functionalized, in order to tune pore size and pore surface property. Different examples of the separation properties will be shown and also the potential use as a membrane reactor will be discussed.

Topical Talk CPP 51.4 Thu 16:45 ZEU/LICH
Molecular electronic materials and devices for solar energy conversion — •Jenny Nelson — Imperial College London

To maximize the potential of solar power, new materials will be needed to harvest and convert solar energy alongside existing photovoltaic technologies. Molecular electronic materials, such as conjugated polymers and molecules, can achieve photovoltaic conversion through a process of photon absorption, charge separation at a heterojunction, and charge collection. Through a remarkable series of advances in materials design, the efficiency of photovoltaic energy conversion in molecular materials has risen from 1% to over 20% within two decades. We will discuss the factors that control the function of molecular solar cells including the nature of the charge separating heterojunction, and the impact of chemical and physical structure on phase behaviour, energy and charge transport, light harvesting, and loss pathways, comparing experimental measurements with a computational model of the generation and evolution of excited states and charges in such systems. We identify key molecular parameters that are likely to assist charge generation and consider the extent to which these parameters are optimised in the best performing materials. Finally, we will address the limits to conversion efficiency in such systems.

Topical Talk CPP 51.5 Thu 17:15 ZEU/LICH
Control of cell and tissue stiffness by biopolymer networks and particle inclusions — •Paul Janmey — University of Pennsylvania, Philadelphia, PA, USA

Filamentous networks of semiflexible polymers are ubiquitous in biology. Collagen fibers form much of the extracellular matrix, the cytoskeleton controls cell mechanics, and chromatin fibers span the volume of the nucleus. The mechanical properties of the biopolymer fibers, the way in which the fibers link into networks, and the types of cells within the network all affect the way in which tissues respond to mechanical stress.

CPP 52: Members' Assembly

Time: Thursday 18:00–19:00 Location: ZEU/LICH

All members of the Chemical and Polymer Physics Division are invited to participate.

CPP 53: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VII

Time: Friday 9:30–11:15 Location: ZEU/LICH

Invited Talk CPP 53.1 Fri 9:30 ZEU/LICH

Limits and Prospects of Organic Solar Cells — •Dieter Neher — Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str 24-25, 14476 Potsdam

Since the advent of low bandgap non-fullerene acceptors (NFAs), the performance of organic solar cells (OSCs) has improved significantly, with record efficiencies that now safely exceed 20 %. A critical parameter is the offset between the relevant frontier orbitals at the DA heterojunction, which in most NFA-based blends is the difference in HOMO energies. Here we combine a wide range of methods, from femtosecond transient absorption to steady state photoluminescence and electroluminescence, spectroscopy to study the mechanisms and efficiency of free charge generation and recombination. For a wide series of NFA-based OSCs, we find that the singlet exciton decay is the main competing pathway for free charge generation while reformation of singlet excitons from reformed CT states dominates the radiative recombination in EL. To explain our data as function of the HOMO offset, we set up a 5-state model which includes singlet and triplet excitons. Our results show that state-of-the-art OSCs already exhibit an optimum HOMO-HOMO-offset. Future work should, therefore, focus on optimizing photon harvesting and reducing bimolecular recombination in order to push the device efficiency well beyond 20 %.

CPP 53.2 Fri 10:00 ZEU/LICH

Temperature Degradation of Slot-Die Printed Organic Solar Cells — •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, Garching, Germany — [2]Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, Trieste, Italy

Organic solar cells (OSCs) have emerged as promising candidates for next-generation photovoltaics due to their rapid efficiency improvements, low toxicity, and compatibility with low-cost, solution-based fabrication methods such as slot-die printing. Their high optical absorption, combined with their lightweight and flexible design, makes them particularly attractive for space applications. Offering a superior power-to-weight ratio compared to conventionally used III-V multijunction cells, OSCs can significantly reduce manufacturing and launch costs. While short-term demonstrations have confirmed their functionality in space, their long-term stability under extreme temperatures, high vacuum, and ionizing radiation still needs to be investigated. Therefore, this study compares the influence of constant-temperature conditions on active-layer morphology and electrical performance with that of temperature cycling. To investigate the degradation process, we employed operando grazing-incidence small-angle X-ray scattering (GISAXS), a nondestructive technique for probing thin-film morphology. Simultaneously, we monitored the electrical performance of the devices under vacuum to simulate space conditions.

CPP 53.3 Fri 10:15 ZEU/LICH

Electronic coarse-graining for accurate and scalable modeling of organic semiconductors — •Andriy Zhugayevych[1], Denis Andrienko[1], and Sergei Tretiak[2] — [1]Max Planck Institute for Polymer Research — [2]Los Alamos National Laboratory, USA

Modeling the electronic properties of organic semiconductors remains challenging due to their complex multiscale structure, which limits the applicability of methods developed for small-molecule solids and inorganic crystals. Fragmentation techniques designed for biomolecular systems are unsuitable for π-conjugated materials because of wavefunction delocalization. We present an electronic coarse-graining methodology that enables accurate and scalable electronic-structure calculations for organic semiconductors composed of monomers with closed-shell π-systems, allowing complete fragmentation along σ-bonds. The approach is demonstrated for crystalline polymers, highlighting how side-group modifications influence the electronic properties of thiophene-based systems such as polythiophene, P3HT, and PEDOT [1]. We further analyze errors introduced by oversimplified electronic models using examples of large flexible molecules, including non-fullerene acceptors for solar cells [2] and OLED materials. The approach can be applied - albeit in less automated way - to broader class of semiconductors, including metal-organic polymers [3], frameworks, and some inorganic semiconductors [4].

[1] Preprint at https://cmsos.github.io/escp; [2] J. Chem. Phys. 159, 024107 (2023); [3] Chem. Sci. 13, 8161 (2022); [4] J. Phys. Chem. Lett. 12, 4674 (2021).

CPP 53.4 Fri 10:30 ZEU/LICH

Facile Correction Method for DFT Band Structures Towards Hybrid Density Functional Level for 2D-Covalent Organic Frameworks — •Laura Fuchs, Maximilian F. X. Dorfner, Matthias Knechtges, Johann Olbrich, and Frank Ortmann — Department of Chemistry, TUM School of Natural Sciences, and Atomistic Modeling Center, Munich Data Science Institute, Technical University of Munich, Germany

Density functional theory (DFT) is the method of choice for predicting the majority of structural, and electronic properties of organic and inorganic materials. Generalized gradient approximations, such as the semi-local PBE functional, are widely used in the community but have one major drawback: the band gap problem. The fundamental band gap is typically underestimated by up to a factor of two by these approaches, which is critical since this electronic property is of utmost importance for assessing the applicability of the investigated material for (opto-)electronic purposes.

Here, we establish a robust linear correlation between the semi-local PBE band gaps and the more accurate, but more expensive, hybrid HSE06 band gaps by analyzing organic molecules as well as extended crystals such as covalent organic frameworks (COFs). By eliminating the need for costly hybrid functional calculations, our approach achieves up to a 54-fold speedup compared to conventional HSE06 computations. We compare various implementation strategies and evaluate each method's advantages and limitations, with particular focus on their implications for predicting electronic transport properties.

CPP 53.5 Fri 10:45 ZEU/LICH

The influence of vibrations on charge and energy transfer dynamics 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 in molecular materials transforming a singlet excited electronic state to two triplet states [1], effectively doubling the number of charge carriers. This makes molecules exhibiting singlet fission possible candidates to increase the efficiency of solar cells beyond the Shockley-Queisser limit. To investigate this possibility, we analyse the charge and energy transfer dynamics in a donor-acceptor complex consisting of a bis(diazadiborine)-based chromophore [2] and tetracyanoquinodimethane. Using a combined approach of *ab initio* multireference perturbation theory calculations and quantum dynamical simulations based on a harmonic vibronic coupling Hamiltonian [3], we reveal competing charge and energy transfer mechanisms, such as singlet fission-based transfer and energy decay channels. Further, we expand our model Hamiltonian to include all vibrational degrees of freedom and the anharmonicity in the vibrational modes of the chromophore. The use of mixed quantum-classical approaches allows us to analyse the influence of these vibrational modes on the dynamics as well as the charge and energy transfer mechanisms.

[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. Chem. Phys.* **151**, 044307 (2019).

CPP 53.6 Fri 11:00 ZEU/LICH

Tracking the degradation of non-fullerene organic solar cells in fluctuating environments — •Lixing Li, Thomas Baier, Xiaojing Ci, Zhaonan Jin, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

The long-term operational stability of non-fullerene organic solar cells (OSCs) remains a critical challenge that limits practical applications. While substantial efforts have been devoted to understanding the degradation mechanisms of OSCs under extreme conditions such as high or low temperatures, far less attention has been paid to their potential recovery behaviour. In real-world environments, organic solar cells are not exposed to constant stress; instead, environmental factors such as temperature, humidity, and illumination fluctuate continuously over time. These dynamic variations may induce partial or even reversible changes in device performance and morphology. It is essential to explore not only how OSCs degrade under stress but also how they recover once the stress is relieved or altered. In this study, we investigate the recovery processes of BTP-4F non-fullerene organic solar cells subjected to multiple environmental parameters. Advanced characterisation techniques, including grazing-incidence X-ray scattering (GIXS) and atomic force microscopy (AFM), are employed to track both in-situ and ex-situ structural evolution within the active layer. These analyses provide new insights into the mechanisms governing the recovery and structural reorganisation of OSCs under dynamic environmental conditions.

CPP 54: Gels, Polymer Networks and Elastomers II

Time: Friday 9:30–11:15 Location: ZEU/0255

Invited Talk CPP 54.1 Fri 9:30 ZEU/0255

NMR-based molecular rheology and structural characterization of model gels — •Kay Saalwächter and Bidit Lamsal — Institut für Physik - NMR, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

Low-resolution proton NMR holds great potential for the routine assessment of the relation between the NMR-detected monomer-level mobility and the relevant physical properties of polymer-based materials. In elastomers and gels, multiple-quantum (MQ) NMR allows for the precise measurement of residual dipolar couplings (RDCs) among the monomer protons, which reflects the conformational space of the highly mobile network chains. In this way, not only the average network chain length but also structural inhomogeneities become accessible. In model networks made by end-linking of star polymers, we can go as far as quantifying connectivity motifs in gels made by heterocomplementary [1,2] and homocomplementary coupling reactions [3], either in one-component [1,3] or amphiphilic co-networks [2].

While the measured RDC is consistently found to be proportional to the gels' elasticity modulus [3], the absolute-level interpretation of the measured average RDC to predict the modulus remains a challenge. We here report on recent experiments performed on a variety of PEO-based model gels to elucidate the effects of solvent on local conformational fluctuations, thermodynamic aspects (solvent quality) and the inhomogeneity of the gels.

[1] Macromolecules 44, 9666 (2011); [2] Macromolecules 55, 6573 (2022); [3] Macromolecules 57, 3058 (2024)

CPP 54.2 Fri 10:00 ZEU/0255

Characterization of the deformation and fracture of tough double-network hydrogels — •Eric Euchler[1], Sitao Wang[2], Konrad Schneider[1], and Sven Wiessner[1,3] — [1]Leibniz-Insititut für Polymerforschung Dresden, Dresden, Germany — [2]Leibniz-Insititut für Polymerforschung Dresden, Dresden, Germany — [3]TUD Dresden University of Technology, Dresden, Germany

Double-network hydrogels (DNHs) feature two interpenetrating networks: a stiff, densely crosslinked first network that carries the load at low strain, and a flexible, loosely crosslinked second network that remains deformable under high strain, offering mechanical properties comparable to elastomers and soft load-bearing biological tissues. Additionally, a yielding phenomenon accompanied by necking of the sample can be observed. This necking zone forms under uniaxial tension and grows with continued loading, which is associated with the fracture of the first network. In this contribution, new insights into the mechanical deformation and damage behavior are given by advanced characterization approaches.

CPP 54.3 Fri 10:15 ZEU/0255

The Role of Connectivity Defects in Governing the Rheology and Microstructure of tPEG Networks — •Sayam Bandyopadhyay[1,2], Sebastian Seiffert[3], and Arash Nikoubashman[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, Germany — [3]Institut für Physikalische Chemie, Johannes Gutenberg-Universität, Germany

We utilized coarse-grained molecular simulations to examine how connectivity defects influence tetra-PEG (tPEG) polymer networks. Both homoleptic and heteroleptic systems were studied, with noncovalent end-group bonds modeled by an inverted Gaussian potential to control valency. Defects were introduced either by deactivating functional end groups or by deviating from ideal stoichiometry in heteroleptic mixtures. Post-gelation structure was quantified using structure factors, radial distribution functions of attractive beads, and internal loop statistics. Network dynamics and molecular mobility were assessed through mean-square displacements of individual tPEG molecules and through bond lifetimes. Our results show that defects enhance loop formation and substantially increase star-polymer mobility. As a consequence, networks with higher defect concentrations exhibit lower viscosity and faster stress relaxation. We also discuss the system's shear response simulated using a mesoscale solvent with hydrodynamic interactions to probe loop and link interconversion kinetics. These findings provide a molecular level understanding of how defects control the structure, dynamics, and mechanical properties of tPEG networks.

CPP 54.4 Fri 10:30 ZEU/0255

Assembling a true Olympic gel from >16,000 combinatorial DNA rings — Sarah K. Speed[1,2], Yu-Hsuan Peng[1,2], Azra Atabay[1,2], Krishna Gupta[1,2], Toni Müller[3,4], Carolin Fischer[5], Ilka Hermes[6], Jens-Uwe Sommer[3,4,7], Michael Lang[3], and •Elisha Krieg[1,2] — [1]Division of Polymer Biomaterials Science, Leibniz Institute of Polymer Research Dresden, Germany — [2]Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Germany — [3]Division of the Theory of Polymers, Leibniz Institute of Polymer Research Dresden, Germany — [4]Institute for Theoretical Physics, Technische Universität Dresden, Germany — [5]B CUBE - Center for Molecular Bioengineering, Technische Universität Dresden, Germany — [6]Division of Physical Chemistry and Physics of Polymers, Leibniz Institute of Polymer Research Dresden, Germany — [7]Cluster of Excellence Physics of Life, Technische Universität Dresden, Germany

Olympic gels consist of a three-dimensional network of mechanically interlocked cyclic molecules providing unique mechanical properties. We report the successful assembly of a true Olympic gel from a library of DNA rings comprising more than 16,000 distinct molecules. Each of these rings contains a unique sequence domain that can be enzymatically activated to produce reactive termini that favor intramolecular cyclization. Results are shown on the genetic, mechanical, and structural characteristics of the material by next-generation sequencing, oscillatory rheology, large-scale computational simulations, atomic force microscopy, and cryogenic electron microscopy.

CPP 54.5 Fri 10:45 ZEU/0255

On the symmetry breaking between gelation and network degradation — •Michael Lang — Division of the Theory of Polymers, Leibniz Institute of Polymer Research Dresden, Germany

Recent experiments indicate that there is a possible symmetry breaking between gelation and network degradation processes in contrast to the predictions of percolation models and classical mean field models. We analyze this problem by large scale computer simulations and mean field modeling in order to avoid possible problems of the experimental setup. The modeling is generalized to capture the main effects of cyclization and composition fluctuations on the gelation process. Both our modeling and the simulation data confirm the existence of the symmetry breaking already for systems above the overlap threshold. This indicates some general problems of the percolation approach for modeling polymer networks.

CPP 54.6 Fri 11:00 ZEU/0255

Crosslinking Mechanisms of Alginate-based Graft Copolymers with Thermoresponsive Side Chains — •Wenqi Xu[1], Sofia-Falia Saravanou[2], Yefan Song[1], Yandong Wang[1], Joachim Kohlbrecher[3], Constantinos Tsitsilianis[2], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]University of Patras, Greece — [3]PSI, Villigen, Switzerland

Alginates are naturally occurring, non-toxic polysaccharides which have seen extensive use in biomedicine. Here, we investigate an alginate-based graft copolymer, namely alginate-*g*-P(NIPAM$_{94}$-*co*-

N*t*BAM$_6$), where a random copolymer of *N*-isopropylacrylamide (NIPAM) and *N*-*tert*-butyl acrylamide (N*t*BAM) is grafted onto a sodium alginate backbone [1]. While introducing thermoresponsive PNIPAM enables temperature-induced gelation, the hydrophobic comonomer N*t*BAM regulates the transition temperature and the mechanical properties of the hydrogel. The structure and the gelation mechanisms of the copolymers are studied in aqueous solutions using small-angle neutron scattering (SANS). At this, contrast matching of the backbone and the side chains was used to obtain selective information. The SANS data show strong forward scattering above the transition temperature of PNIPAM, which is attributed to the collapse of the side chains, resulting in hydrophobic globules which act as nodes of the hydrogel network.

[1] K. Safakas, C. Tsitsilianis. *Int. J. Mol. Sci.* **2021**, 22(8), 3824.

CPP 55: Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates III (joint session CPP/BP)

Time: Friday 9:30–11:15 Location: ZEU/0260

Topical Talk CPP 55.1 Fri 9:30 ZEU/0260

Data-driven modelling of phase-separating intrinsically disordered regions — •Giulio Tesei[1,2], Fatima Kamal Zaidi[3], Shanlong Li[4], Julian O. Streit[1], Jianhan Chen[4], Tanja Mittag[3], and Kresten Lindorff-Larsen[1] — [1]Department of Biology, University of Copenhagen, Copenhagen, Denmark — [2]Department of Biomedical Science, Malmö University, Malmö, Sweden — [3]Department of Structural Biology, St. Jude Children's Research Hospital, Memphis, U.S.A. — [4]Department of Chemistry, University of Massachusetts, Amherst, U.S.A.

Intrinsically disordered regions (IDRs) constitute about one third of the human proteome and play important roles in biological processes. While lacking well-defined 3D structures, IDRs adopt heterogeneous ensembles influenced by multivalent interactions; these same interactions can promote phase separation and contribute to the formation of biomolecular condensates. I will first present CALVADOS, an efficient one-bead-per-residue model optimized on experimental data reporting on IDR conformational properties and extensively validated on both single-chain and phase behavior across diverse sequences. I will then describe how we used large sets of CALVADOS simulations to train machine-learning models that accurately predict single-chain compaction and homotypic phase-separation propensity directly from sequence. Finally, I will introduce a hybrid-resolution model with an atomistic backbone representation that matches the accuracy of CALVADOS for global dimensions and phase separation while also capturing local structure and backbone hydrogen bonding.

CPP 55.2 Fri 10:00 ZEU/0260

Born to Condense: Polysomes Drive Co-Translational Condensation of Biomolecular Condensate Proteins — •Zhouyi He, Jens-Uwe Sommer, and Tyler Harmon — Leibniz Institute of Polymer Research, 01069, Dresden, Germany

Biomolecular condensates formed by protein LLPS are ubiquitous and crucial in cells. While the physics and functions of LLPS are well studied, its interplay with protein synthesis, translation, remains largely unexplored. Here we propose Co-Translational Condensation (CTC), a mechanism in which nascent protein chains of polysomes, multiple ribosomes on one mRNA, interact with condensates, localizing translation to condensate surfaces. Using coarse-grained simulations, we show that protein domain architecture dictates the extend of CTC, consistent with a Langmuir adsorption model. Bioinformatic analysis reveals that most condensate-associated proteins have architectures favoring CTC, with strong interaction regions of nascent chains exposed on polysomes. Dynamically, simulation and reaction-diffusion modeling reveal that CTC is kinetically feasible within typical polysome lifetimes, either through large polysomes nucleating new condensates or via diffusion to pre-existing condensates. As a case study, we demonstrate that CTC enhances post-translational modifications by minimizing unmodified intermediates. More broadly, we anticipate CTC may also influence protein folding, misfolding, and signal-integration latency. Together, our results establish CTC as a general mechanism coupling translation with phase separation, with broad implications for protein evolution, cellular organization, and synthetic biology.

CPP 55.3 Fri 10:15 ZEU/0260

Local RNA/protein stoichiometry tunes the electrostatic microenvironment inside reconstituted multicomponent condensates — •Patrick M. McCall — Leibniz Institute for Polymer Research Dresden, Dresden, DE

Biomolecular condensates are demixed phases of biopolymers and, in living cells, commonly form through the associative phase separation of strongly-charged nucleic acids together with protein polyampholytes carrying a weak net charge. While condensates are proposed to offer distinct aqueous environments for the organization of cellular biochemistry, it remains unclear which physical aspects of the microenvironment are relevant and how widely they can vary between condensates. Motivated by the large asymmetry in structural charge between typical condensate components such as RNAs and RNA-binding proteins, we explore here the implications of electroneutrality on the electrostatic environment within model multicomponent condensates. Combining classical Donnan theory with recent measurements of the macromolecular composition of condensates reconstituted from full-length FUS protein and a homopolymeric RNA [McCall et al Nat Chem 2025], we compute the partitioning of salt ions as well as the Donnan potential across the phase boundary. We find that RNA/FUS stoichiometry tunes both co-ion exclusions over a wide range and is coupled to a pH jump across droplet interface. We also find that co-ion exclusion is suppressed by counter-ion condensation and enhanced by non-ideality of un-bound ions. These results provide insight into the range of ionic conditions accessible to a prominent class of biomolecular condensate.

CPP 55.4 Fri 10:30 ZEU/0260

Coarse-grained model to study the effects of electric fields on protein interactions — •Agaya Johnson[1], Debes Ray[2,4], Mahnoush Madani[3], Jan Dhont[2,3], Florian Platten[2,3], Kyongok Kang[2], and Sofia Kantorovich[1] — [1]University of Vienna, Kolingasse 14-16, 1090, Vienna, Austria. — [2]nstitute of Biological Information Processing IBI-4, Forschungszentrum Jülich, 52428 Jülich, Germany. — [3]Faculty of Mathematics and Natural Sciences, Heinrich Heine University Düsseldorf, 40225 Düsseldorf, Germany. — [4]Solid State Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400085, India.

Proteins can undergo transition between a wide range of organisational states, from soluble monomers to disordered phases and ordered structures. Experiments have shown that lysozyme in sodium thiocyanate solution can form homogeneous, crystalline, or liquid phases depending on the salt and protein concentrations, and that these phase boundaries can be shifted by applying an electric field. We present a coarse-grained model of lysozyme in sodium thiocyanate solution, representing the protein as an ellipsoid decorated with charged and adhesive surface patches. Counterions and monovalent salt are treated explicitly via excluded-volume repulsion and Coulombic interactions. We investigate (i) how patch size and salt*patch interactions influence ion distributions around a single protein, with and without an external electric field, and (ii) the resulting effective interactions between two proteins as functions of patch properties, salt concentration, and applied electric field.

CPP 55.5 Fri 10:45 ZEU/0260

Entropic Clustering of Stickers Induces Aging in Biocondensates — •Hugo Le Roy[1] and Paolo De Los Rios[2] — [1]Department of Civil, Chemical and Environmental Engineering, University of Genoa, Genoa, Italy — [2]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne

Neurodegenerative conditions, such as Parkinson's disease, results from the aggregation of synaptic proteins such as alpha-synuclein. In a healthy presynaptic neuron, effective neurotransmission relies on the spatial organization of synaptic vesicles within phase-separated droplets. These vesicles release neurotransmitters into the synaptic cleft to activate ion-gated channels on the postsynaptic neuron.

In this work, we investigate how this transmission process is impaired during neurodegeneration. Specifically, we focus on the solidification of these phase-separated droplets, a phenomenon described as aging, leading to protein aggregation and associated with the emergence of pathology. We explore the connection between the mechanical properties of the condensates and their microscopic structure using a minimal physical model that treats complex molecules as stickers and spacers. We show that entropy maximization of spacers leads to an effective attractive force between stickers. As a result, our system displays a surprisingly slow relaxation toward equilibrium, reminiscent of glassy systems and consistent with the liquid-to-solid transition observed in aging droplets. By analyzing the clustering dynamics of stickers, we successfully explain the microscopic origin of this glassy relaxation.

CPP 55.6 Fri 11:00 ZEU/0260

Biomolecular condensates with a Twist: From Assembly to Arrest — •Mahesh Yadav[1,2] and Lukas Stelzl[2] — [1]Institute of Physics, Johannes Gutenberg University, Mainz — [2]Institute of Molecular Physiology, Johannes Gutenberg University, Mainz

In this work, we investigate the phase behavior of RNA-binding protein Fused in Sarcoma (FUS), whose multivalent and intrinsically disordered regions drive the formation of biomolecular condensates through liquid-liquid phase separation. FUS is a multi-domain protein with arginine-glycine-rich segments (RG-rich domains) that participate in essential cellular proceses. We examine how characteristic sequence motifs such as RGG.. mediate homotypic and nucleic acid binding, and how targeted point mutations (e.g., RtoK, RtoA) disrupt these motifs and impair condensate formation. Using the thermodynamics phase diagram as a benchmark we highlighted the shift in phase separation propensity of the FUS and its variants. Furthermore, we identify the role of key interactions such as electrostatics, π-π and cation-π in nucleic acid binding at atomistic scale. We further characterized the emergent viscoelastic behavior of FUS condensates at multiple scales. We observe that upon mutations the overall dynamics slows down which reflects the gel-like state. Within the condensate interior, protein chains exhibit sub-diffusive dynamics arising from intermittent binding and viscoelastic resistance, mobility at the interface is further suppressed due to anisotropic interactions and interfacial confinement. To quantify these behaviors across relevant scales, we employ multi-resolution simulation models.

CPP 56: Molecular and Polymer Dynamics, Friction and Rheology I

Time: Friday 10:45–12:00 Location: HÜL/S386

Invited Talk CPP 56.1 Fri 10:45 HÜL/S386

Liquid Dynamics at Interfaces — •Michael Vogel — Institut für Physik kondensierter Materie, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt

Liquids at interfaces are of great importance in nature and technology, for instance, in biological cells, clay minerals, and energy materials. Typically, the dynamics of liquids at interfaces significantly differ from those in the bulk. We combine nuclear magnetic resonance and broadband dielectric spectroscopy with molecular dynamics simulutations to determine the magnitude and range of these interface effects in broad frequency and temperature ranges. It is shown that the free energy landscape imposed by an interface on an adjoining liquid enables a basic understanding of the altered dynamical behavior [1]. It will be discussed that a knowledge of interface effects allows one not only to obtain valuable insights into the properties of confined water and, when avoiding crystallization, the anomalies and vitrification of bulk water [2-4], but also to steer ion transport in electrolyte-host systems for improved lithium-ion battery and proton-exchange membrane materials [5-7].

[1] S. Hefner et al., Phys. Rev. Lett. 133, 106201 (2024)
[2] V. Schiller and M. Vogel, Phys. Rev. Lett. 132, 016201 (2024)
[3] J. H. Melillo et al., PNAS 121, e2407030121 (2024)
[4] E. Steinrücken et al., J. Phys. Chem. Lett. 14, 4104 (2023)
[5] M. Stevenson et al., Adv. Funct. Mater. e15706 (2025)
[6] S. F. Winterstein et al., J. Am. Chem. Soc. 145, 27563 (2023)
[7] A. F. Privalov et al., J. Phys. Chem. Lett. 14, 9335 (2023)

CPP 56.2 Fri 11:15 HÜL/S386

The analytical and numerical investigation of star-shaped copolymers with three arms in confined geometries — •Zoriana Danel[1], Joanna Halun[2], and Paweł Karbowniczek[1] — [1]Cracow University of Technology, Poland — [2]Institute of Nuclear Physics, Poland

The influence of star copolymer topology on the depletion interaction potentials, the depletion forces, the radius of gyration and the monomer density profiles is investigated analytically and numerically. The method of analytical calculation of the dimensionless depletion interaction potentials and the dimensionless depletion forces for a dilute solution of ideal star-shaped copolymers with three legs in combination f=2-1 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 is proposed. Besides, molecular dynamic simulations of a dilute solution of star-shaped copolymers in a good solvent with three number of legs with N=801 monomers (300+300+200+1) for combination f=2-1 and N=701 monomers (300+200+200+1) for combination f=1-2 confined in a slit with different boundary conditions are performed and the results of the monomer density profiles for the above mentioned cases are obtained for the narrow and wide slit region. Furthermore, the numerical calculations of the radius of gyration for star-shaper copolymers in combination f=2-1 and f=1-2 are performed. The obtained results are interesting from scientific and practical point of view, because of their potential application in materials engineering, nano-technology, biotechnology and medicine.

CPP 56.3 Fri 11:30 HÜL/S386

Polymer melt dynamics in the light of viscoelastic hydrodynamic interaction — •Hendrik Meyer — Institut Charles Sadron, Université de Strasbourg, CNRS UPR22, 67034 Strasbourg, France

Our group has shown that anomalous center-of-mass (CM) diffusion occurring on intermediate time scales in polymer melts can be explained by the interplay of viscoelastic and hydrodynamic interactions (VHI). The theory has been solved for unentangled melts in 3D [1] and 2D [2] and excellent agreement between theory and molecular dynamics simulation is found. The theory was developed for momentum conserving dynamics as well as Langevin dynamics. The physical mechanism considers that hydrodynamic interactions are time dependent because of increasing viscosity before the terminal relaxation time. We show that this mechanism is generally active and relevant in melts including entangled systems, rings or stars.

[1] PRL 107, 178301 (2011); PRE 85, 051807 (2012). [2] PRL 109, 248304 (2012); Soft Matter 9, 4249 (2013).

CPP 56.4 Fri 11:45 HÜL/S386

Knots in Polymers under Shear Flow — •Maurice P. Schmitt[1], Andrey Milchev[2], and Peter Virnau[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany — [2]Institute of Physical Chemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria

Knots in polymers and biological macromolecules, such as DNA and proteins, are crucial to their structure and function. However, the effect of external forces on knots in polymers is still insufficiently understood. Here, we investigate the impact of shear and Poiseuille flow on knotted flexible polymers using Molecular Dynamics (MD) and Multi-Particle Collision Dynamics (MPCD) simulations. We find that under simple shear (Couette flow), initially loose knots in polymer coils tighten beyond a critical shear rate. Further increase of the shear rate leads to tumbling motions of the chains in flow and fluctuating knot sizes. In contrast, knotted polymer globules subjected to shear unfold into pearl-necklace-like conformations, whereby knots spread across multiple sub-globules and undergo dynamic topological transitions. In Poiseuille flow, knots also tighten under increasing flow strength, with fluctuations in knot size emerging at high shear rates. Unexpectedly, the slit thickness significantly influences the tightening process even at constant mean shear rate. These findings reveal that both Couette and Poiseuille flow induce major structural and topological transformations in knotted polymers, offering insight into the behavior of knots under hydrodynamic forces in confined and driven environments.

CPP 57: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VIII

Time: Friday 11:30–13:00 Location: ZEU/LICH

CPP 57.1 Fri 11:30 ZEU/LICH

Novel n-Dopants for Improving Organic Solar Cells — •Yahya Asl Soleimani[1], Nora Engelmann[1], Stephanie Buchholtz[1], Jörn Vahland[2], Adrian Kishonti[2], Steffen Woltering[2], Karl Leo[1], and Johannes Benduhn[1] — [1]Institute of Applied Physics, Technische Universität Dresden, Nöthnitzer Straße 61, 01187 Dresden, Germany — [2]CREDOXYS GmbH, Liebigstraße 26, 01187, Dresden, Germany

Doping is a crucial concept in semiconductor technology, and it is no different for organic semiconductors. It increases conductivity and facilitates carrier injection and extraction. While substantial success has been achieved for organic molecular p-dopants, the same cannot be said for n-dopants. They suffer from an inherent disadvantage: the highest occupied molecular orbital (HOMO) of the n-dopant must be lower than the lowest unoccupied molecular orbital (LUMO) of the host, rendering them typically unstable under ambient conditions. Here, we report a new and efficient molecular n-dopant that can dope C_{60} to a conductivity of 20 S/cm. We investigate the origin of its efficacy and explore the doping mechanism using ultraviolet electron spectroscopy (UPS). Moreover, we incorporate the new n-dopant into organic solar cells, demonstrating its effectiveness by improving the power conversion efficiency of the reference devices.

CPP 57.2 Fri 11:45 ZEU/LICH

Computational Study of Electronic Trapping in TADF Host-Guest Systems — •Naomi Kinaret[1], Andrei Stankevych[2,3], Andriy Zugayevych[1], Rishabh Saxena[1], Alexander Vakhnin[3], Kun-Han Lin[1,4], Denis Andrienko[1], Heinz Bässler[2], Anna Köhler[2], and Andrey Kadashchuk[2,3] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]University of Bayreuth, Bayreuth, Germany — [3]National Academy of Sciences of Ukraine, Kyiv, Ukraine — [4]National Tsing Hua University, Hsinchu, Taiwan

Extrinsic traps created by dopants or impurities are ubiquitous in organic semiconductors and can critically influence charge transport [1]. Here we report a computational study of the trapping of charge carriers in amorphous host-guest systems of the thermally activated delayed fluorescence (TADF) emitter DMAC-TRZ in two different hosts, validated by low-temperature thermally- stimulated luminescence (TSL). In both hosts we find that DMAC-TRZ forms an additional Gaussian density of states (DOS), offset from the host DOS by a trap depth ϵ_t. In both systems trap depths and DOS widths, σ_{DOS}, agree with experimentally observed values over a range of compositions, showing that the nominal trap depth is concentration independent. In the case of deep traps, $\epsilon_t > 3\sigma_{DOS}$, we observe concurrent charge detrapping via guest-to-host and guest-to-guest pathways, with the latter dominating for $c_t > 5\%$. Guest-guest transfers are observed already at the low guest concentration of $c_t = 1\%$, attributed to local guest clustering and superexchange- mediated inter-cluster transfers.

[1] Kotadiya, N.B., et al., Nat. Mater. (2019).

CPP 57.3 Fri 12:00 ZEU/LICH

Interface Engineering toward High-Performance Subphthalocyanine-based Single-Component Organic Photodetectors — •Anncharlott Kusber[1], Ying Sun[2], Jakob Wolanksy[1,3], Fred Kretschmer[1], Conrad Winkler[1,3], Anna-Lena Hofmann[1], Ji-Seon Kim[2], Karl Leo[1], and Johannes Benduhn[1,3] — [1]Institute of Applied Physics, Technische Universität, Dresden, Germany — [2]Imperial College London, United Kingdom — [3]German Centre of Astrophysics, Görlitz, Germany

Organic photodetectors (OPDs) have attracted considerable attention due to their capability to convert light into electrical signals and enable high-quality imaging, while simultaneously offering the intrinsic benefits of organic materials. Single-component (SC) OPDs, using a single photoactive organic semiconductor material, have several advantages over the commonly used bulk heterojunction OPDs such as its simplified structure. The influence of several organic electron transport layers (ETLs) on energetic landscape at the immediate interface with organic layers has not yet been systematically reported. This is necessary to gain a deeper understanding of physics of organic interfaces, thereby enabling the further optimization of OPD performance. Sensitive measurement techniques were used to analyse the influence of different organic interfaces on the OPD performance.

These investigations lead to SubNc SC OPD devices, which achieves an EQE of 56 % at 0 V, an ultra-low J_D of $2.5 \cdot 10^{-11}\,\mathrm{A} \cdot \mathrm{cm}^{-2}$ at -0.5 V and D* of $3.8 \cdot 10^{14}$ Jones at 0 V (based on calculated shot noise).

CPP 57.4 Fri 12:15 ZEU/LICH

Impact of additive on the morphology and electronic states of PPDT2FBT:PCBM organic solar cells — Md Moidul Islam[1,2], Hassan Ismail[1,2], Saib Qazi[1,2], Ulrich S. Schubert[1,2], and •Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstrasse 10, 07743 Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

Among organic solar cells using PCBM as an acceptor, the donor PPDT2FBT yields one of the highest power conversion efficiencies (PCE) of nearly 10%. It has been demonstrated that the processing additive diphenyl ether (DPE) contributes to that success essentially. However, the exact mechanism responsible for the performance improvement has so far not been revealed. Therefore, we undertook a systematic study for comparing PPDT2FBT:PCBM solar cells, under variation of annealing temperatures and use of DPE. A combination of optical, electrochemical, microscopic, and further characterization methods enabled the decoding of the impact of DPE on the blend morphology. In addition, the limitation in device stability by extended morphological degradation has been revealed and strategies to overcome those are being discussed.

CPP 57.5 Fri 12:30 ZEU/LICH

Photo-physics of symmetric and asymmetric ITIC-2F nonfullerene acceptors in organic solar cells — •Shahidul Alam[1,2], Nisreen Alshehri[2], Michael Bulgakov[3], Zerui Li[4], Khawla Alkhezaim[2], Maryam Alqurashi[2], Oleksandr Matiash[2], Vojtech Nadazdy[5], Martin Hager[6], Ulrich S Schubert[6], Vladimir Dyakonov[3], Harald Hoppe[6], Peter Müller-Buschbaum[4], Andreas Sperlich[3], and Frédéric Laquai[1,2] — [1]LMU Munich — [2]KAUST, Saudi Arabia — [3]University of Wurzburg — [4]TU Munich — [5]Slovak Academy of Sciences, Slovak Republic — [6]FSU Jena

Fluorination is an effective strategy to tune the electronic and structural properties of organic semiconductors by lowering frontier orbital energies, enhancing intermolecular interactions, and improving stability. We investigated ITIC and its fluorinated derivatives, sITIC-2F and aITIC-2F, in blends with PBDB-T and its halogenated analogue PM6 to elucidate the effects of fluorination on molecular packing and energetics. Optically detected magnetic resonance reveals triplet excitons in all pristine materials and blends, with their donor-acceptor distribution governed by fluorination. These results demonstrate that fluorination effectively modulates molecular organization and excited-state dynamics, leading to improved structure-property-performance relationships in organic solar cells.

CPP 57.6 Fri 12:45 ZEU/LICH

Single-Component Vacuum-Deposited Organic Photodetectors Achieving NIR Detection — •Jakob Wolansky[1,4], Jacob Hille[1], Cedric Hoffmann[2], Michel Panhans[3], Frank Ortmann[3], Natalie Banerji[2], Karl Leo[1], and Johannes Benduhn[1,4] — [1]IAPP, TU Dresden, Germany — [2]DCBP, University Bern, Switzerland — [3]NAT-School, TU Munich, Germany — [4]DZA, Görlitz, Germany

Efficient charge separation in organic semiconductor devices typically relies on an energetic offset at the donor-acceptor interface to dissociate photogenerated electron-hole pairs. While such an offset facilitates charge generation, it can limit the maximum open-circuit voltage. Additionally, interfacial traps generate charge carriers in the dark. To address these limitations, significant research is exploring single-component (SC) architectures that minimize interfacial losses.

In this work, we investigate SC organic photodetectors in which a newly developed small molecule serves as the active layer. By chemically tuning the molecular structure, extended near-infrared absorption up to 900nm is achieved, while maintaining devices with a large linear dynamic range of 160dB, a -3dB cutoff frequency of 50kHz, and an external quantum efficiency of 20% at zero bias. Comparison with the widely studied small molecule DCV2-5T allows the extraction of structure-property relationships that serve as a basis for future molecular design. Furthermore, an in-depth analysis of the charge generation process in DCV2-5T provides new insights into the pathways governing efficient photogeneration in SC organic systems.

CPP 58: Gels, Polymer Networks and Elastomers III

Time: Friday 11:30–13:00 Location: ZEU/0255

CPP 58.1 Fri 11:30 ZEU/0255

X-ray induced structural changes in supramolecular polymer networks — •Niels C. Giesselmann[1,2], Yasothaa Thavayogarajah[3], Mostafa Ahmadi[3], Sebastian Seiffert[3], and Katrin Amann-Winkel[1,2] — [1]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany — [3]Institute of Chemistry, Johannes Gutenberg University, Mainz, Germany

Supramolecular polymer networks consist of non-covalently crosslinked macromolecules. Such transient links can be established through functionalized polymer building blocks. An interesting property of this group of materials is their ability to self-heal mechanical damage. We observed polymer networks made of star-shaped four-arm PEG building blocks with metal-complexing end groups. Due to their transient binding, the building blocks diffuse through the polymer network in a process that is not yet understood in detail. In this study, we employed both X-ray scattering in order to probe the structure of the network on the molecular as well as the macromolecular level. This way, we hope to better understand the mechanical and self-healing properties of these polymer networks. We report the emergence of structural changes in dependence of the X-ray flux that futhermore persist when measuring far away from the initially illuminated area. This effect can be explained by the affected molecules spreading throughout the sample by means of the transient binding dynamics mentioned above.

CPP 58.2 Fri 11:45 ZEU/0255

Deciphering the photopolymerization-induced nanostructure and interface formation for submicron additive manufacturing — •Shouzheng Chen[1,2,3], Yufeng Zhia[2], Lixing Li[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, Garching, Germany — [2]DESY, Hamburg — [3]MLZ, TUM, Garching, Germany — [4]TU/e, Eindhoven, the Netherlands — [5]Covestro (Netherlands) B.V., Geleen, the Netherlands — [6]Department of Fibre and Polymer Technology, KTH, Stockholm, Sweden

UV-curing is widely used in additive manufacturing due to its controllable spatiotemporal characteristics. In submicron additive manufacturing, the involvement of solvents and limitations on film thickness complicate the precise regulation of nanostructures and interlayer interface. By using grazing incidence small angle X-ray scattering (GISAXS) and employing the oligomer (urethane dimethacrylate, UDMA)/monomer (2-ethylhexyl acrylate, 2-EHA) based resin system, we quantify the heterogeneous distribution of UDMA- and 2-EHA-rich nanodomains (around 23 nm and 13 nm in radii, respectively) in the cured system. Combining Bornagain, we reveal the buried "frozen" nano-wrinkles at interlayer interfaces(cones with radius of 70 nm, slope angle of 18°) induced by solvent and constraint stress synergistically. Our findings offer deeper insights for high precision submicron additive manufacturing.

CPP 58.3 Fri 12:00 ZEU/0255

From real polymers to random graphs: percolation thresholds in associative polymer solutions — •Xinxiang Chen, Lennart Hebestreit, and Friederike Schmid — Johannes Gutenberg-University Mainz, Mainz, Germany

Multivalent reversible crosslinking is ubiquitous in soft matter and biomolecular condensates, yet their sol-gel transitions often deviate from the classical Flory-Stockmayer picture due to chain conformations, intrachain binding, and loop formation. Here, we develop a unified framework combining molecular dynamics simulations with random-graph and random-geometric-graph approaches to quantitatively link real polymer architectures to abstract network models. For single- and two-component reversible polymers with one-to-one specific binding, we determine gel points from topological connectivity and find percolation thresholds substantially higher than Flory-Stockmayer predictions. By comparing spatially unconstrained random graphs with spatially correlated random geometric graphs, we show that intrachain binding and loops markedly reduce the effective interchain bonding needed to form an infinite cluster. Meanwhile, the theoretical results of the generating function and the Lagrange inversion further yield cluster size distributions and giant cluster fractions. Our work demonstrates how spatial correlations and polymer conformations fundamentally reshape reversible network formation, offering a unified topological and physical perspective on reversible gels and biomolecular condensates.

CPP 58.4 Fri 12:15 ZEU/0255

From Champagne Fizzling to Confined Polymer: Natural and Artificial Bubble Nucleation — •Carlos Arauz-Moreno[1,2], Keyvan Piroird[2], and Elise Lorenceau[1] — [1]Université Grenoble Alpes, CNRS, LIPhy, F-38000 Grenoble, France — [2]Saint-Gobain Research Paris, F-93360 Aubervilliers, France

Bubbles dazzle the senses when pouring a Champagne glass. However, there is a hidden trick to this elegant experience: natural nucleation sites, such as tartrate crystals from washing or cellulose fibers from drying, or artificial sites, like crenels in the flute, are used to trigger bubble nucleation by lowering the energy barrier required to grow a bubble; otherwise, Champagne wouldn't bubble at all. By using a model system of viscoelastic polyvinyl butyral (PVB), we show that the concepts of natural and artificial nucleation from Champagne equally apply to confined viscoelastic polymers. Our experimental results show that water vapor, which tends to aggregate inside the PVB matrix in the form of clusters, escapes in copious amounts from the polymer bulk when the latter is heated and decompressed (e.g., at 140°C, dP=1bar). However, bubbles may only form at naturally trapped fibers, dust speckles, or in artificial crenels on the glass surface. The number of natural nuclei is apparently and counterintuitively inversely proportional to the applied temperature. Moreover, bubbles can take on different shapes and sizes because coalescence does not occur. Finally, we investigated how the growth rate of bubbles is impacted by whether nucleation is natural or artificial, revealing a clear distinction between the two: the growth rate in the former is global while in the latter is local.

CPP 58.5 Fri 12:30 ZEU/0255

Steric Origins of Microgel Thermoresponsiveness Revealed by All-Atom Polymer Simulations — •Jannis Krüger[1], Letizia Tavagnacco[2], Emanuela Zaccarelli[2], and Thomas Hellweg[1] — [1]Physical and Biophysical Chemistry, Bielefeld University, Germany — [2]Department of Physics, Sapienza University of Rome, Italy

Microgels based on N-isopropylacrylamide (NIPAM) are well established in soft matter science due to their thermoresponsive swelling behavior. Dynamic light scattering (DLS) reveals a sharp decrease in the hydrodynamic radius at a characteristic volume phase transition temperature (VPTT), which occurs around 34°C. In our previous work[1] we observed that by adding a non-thermoresponsive comonomer such as N-tert-butylacrylamide (NtBAM), this transition broadens in temperature until it disappears at high molar contents. The VPT is typically interpreted in terms of hydrophilicity or hydrophobicity; however, the steric demand of chemical substituents is often overlooked. In this work, we compare DLS measurements with all-atom molecular dynamics simulations of NIPAM and NtBAM polymer chains in water, to show how subtle differences, like replacing an isopropyl with a tert-butyl group, substantially affects the coil-globule transition of polymers in water, thereby providing deeper insights into the molecular origin of the broadening and lowering of the VPTT in real microgels.

[1] J. Krüger, S. Kakorin, and T. Hellweg, Colloid Polym. Sci. 303, 1815 (2024).

CPP 58.6 Fri 12:45 ZEU/0255

Photo-responsive microgels as model systems with tunable crosslinking density — •Dominik Wöll and Christian Metzen — Institute of Physical Chemistry, RWTH Aachen University

Functional microgels have powerful applications due to their specific structure, which can quickly respond to external stimuli such as temperature, pH, ionic strength, solvent composition, and light. We synthesized double-responsive poly(N-isopropylacrylamide) (PNIPAM) microgels that react to both light and temperature. The light responsiveness is achieved by the addition of photoswitchable trans-azobenzene (Azo) units that crosslink with the corresponding β-cyclodextrin (β-CD) units copolymerized into the microgel. Irradiation with light causes switching from trans-Azo to cis-Azo and thus opening of the crosslink. With the wavelength of light, and the corresponding photostationary state, the crosslinking density in these microgels can be precisely controlled with light. This model system allows us to investigate the influence of crosslinking density on the structure and properties of microgels.

CPP 59: Crystallization

Time: Friday 11:30–13:00 Location: ZEU/0260

CPP 59.1 Fri 11:30 ZEU/0260

Structure formation in Polyamide 6 under process-relevant conditions: In situ SAXS/WAXS study using a modular FlowCell setup — •Anna Katharina Sambale[1], Eric Euchler[1], Moritz Kurkowski[1], Enno Henn[1], Regine Boldt[1], Matthias Schwartzkopf[2], Sarathlal Koyiloth Vayalil[2,3], and Markus Stommel[1,4] — [1]Leibniz-Institut fuer Polymerforschung Dresden e.V., Dresden, Germany — [2]Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — [3]Applied Science Cluster, UPES, Dehradun, India — [4]TUD Dresden University of Technology, Dresden, Germany

The microstructural evolution of semi-crystalline thermoplastics during melt processing is governed by local thermo-rheological conditions, which strongly influence crystallization kinetics and consequently, the final material properties. To analyze these interdependencies under process-relevant conditions, a modular FlowCell setup was developed for time-resolved in situ SAXS/WAXS experiments at the synchrotron beamline P03 at DESY, Hamburg. The setup combines a commercial single-screw extruder with customized temperature-controlled slit capillary that enables measurements during controlled cooling from the melt to solid state, with synchronized acquisition of IR-thermography data and, in extended configurations, Raman spectroscopy. Recent experiments on polyamide 6 demonstrate the impact of different cooling strategies and nucleation conditions on the resulting structure. The results highlight the relevance of spatially and temporally resolved analysis techniques for understanding structure formation towards industrial polymer processing.

CPP 59.2 Fri 11:45 ZEU/0260

Influence of Composition on Sanidic Liquid Crystalline Mesophases in Statistical Copolythiophenes — •Alexander Much[1], Jakob Danziger[1], Qian Wang[2], Michael Sommer[2], and Oleksandr Dolynchuk[1] — [1]Martin-Luther-Universität Halle-Wittenberg — [2]Technische Universität Chemnitz

Liquid-crystalline (LC) materials exhibit a variety of structural forms depending on the degree of order, allowing for the novel combination of their anisotropic properties. Board-like conjugated polymers with stiff backbones and short side chains, such as poly-(3-hexylthiophene) (P3HT), are of particular interest because they exhibit weakly explored sanidic LC mesophases.

Here, we study the influence of chemical side-chain modification on the LC phase transitions in statistical copolymers poly-(3-hexylthiophene)-stat-poly-[3-(6-cyanohexyl)thiophene] using differential scanning calorimetry (DSC) and temperature-resolved wide angle X-ray scattering. We find that the copolythiophenes go trough a cascade of sanidic LC mesophases during heating, similar to those in P3HT. Remarkably, the temperature range where sanidic mesophases exists follows the melting range from DSC as a function of comonomer composition and increases towards the intermediate composition with an apparent minimum in values of melting temperature and enthalpy. This suggest that energetic contributions reduce the thermal stability of sanidic LC phases in copolythiophenes, and that LC transition temperatures can be tuned through statistical copolymerization without negating their existence.

CPP 59.3 Fri 12:00 ZEU/0260

In-situ structure and morphology investigations of slot-die coated perovskite nanocrystal films — •Thomas Baier[1], Altantulga Buyan-Arivjikh[1], Lixing Li[1], Xiaojing Ci[1], Markus Döblinger[2], Matthias Schwartzkopf[3], Thomas Bein[2], Sarathlal Koyiloth Vayalil[3,4], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Department of Chemistry, LMU, Munich — [3]DESY, Hamburg — [4]UPES, Dehradun

Colloidal perovskite nanocrystals (PNCs) are promising in contributing to next-generation optoelectronic and energy conversion technologies. In this work, mixed-cation cesium-formamidinium lead-iodide (Cs(1-x)FAxPbI3) PNCs were synthesized via a colloidal hot-injection route and subsequently processed into thin-film active layers using slot-die coating for scalable manufacturing. The evolution of structural order during deposition was probed in-situ using grazing-incidence small- and wide-angle X-ray scattering (GISAXS and GIWAXS), providing direct insights into nanocrystal packing, ordering, and defect formation. Simultaneous optical characterization via photoluminescence (PL) provided complementary information on the evolution of optical properties during deposition, while transmission electron microscopy (TEM) enabled correlation with nanoscale information. By combining colloidal synthesis, in-situ structural probes, and optical characterization, this work directly links nanoscale assembly, defect states, and the optoelectronic performance of perovskite nanocrystal thin films.

CPP 59.4 Fri 12:15 ZEU/0260

Interplay of heterogeneous nucleation and prefreezing in PBS droplets on graphene — •Marthinus van Niekerk, Moritz Hartelt, and Oleksandr Dolynchuk — Experimental Polymer Physics, Martin-Luther-University Halle-Wittenberg, Germany

The dominant crystallization mechanism depends on the kinetics of formation and crystal growth. Heterogeneous nucleation, leading to spherulitic morphology, and prefreezing, leading to epitaxial morphology, are two mechanisms of interface-induced crystallization in polymers. However, research on prefreezing is in a seminal phase, and its possible competition with nucleation during cooling remains unexplored. Here, we study the crystallization behavior of dewetted poly(butylene succinate) (PBS) droplets on graphene, a known prefreezing substrate for PE and PCL, during cooling from the melt at different rates using optical- and atomic force microscopy and wide-angle X-ray scattering. Across a large range of cooling rates, nucleation was found to be dominant, resulting in spherulitic morphology in large droplets. However, indications of prefreezing were observed in very small droplets exhibiting epitaxial morphology. Subsequent annealing close to T_m resulted in significant reordering and enhancement of out-of-plane orientation, causing a change in morphology from spherulitic to epitaxial for all droplets up to several hundred nanometers. Theoretical analysis revealed a significant lattice mismatch between graphene and PBS, suggesting it is a plausible reason for the absence of rapid prefrozen layer growth during initial cooling from the melt.

CPP 59.5 Fri 12:30 ZEU/0260

Crystallization of polymer networks in the constant-strain and constant-stress ensembles — Atmika Bhardwaj[1], Huzaifa Shabbir[1], Jens-Uwe Sommer[1,2], and •Marco Werner[1] — [1]Bereich Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, Germany

We investigate how deformation and cross-links affect the crystallization of polymer networks using molecular dynamics simulations. A cooling- and heating cycle are simulated both under constant-strain and constant-stress conditions, monitoring specific volume, crystallinity, and orientational order as functions of temperature. In both ensembles, deformation induces chain pre-alignment along the loading direction, driving crystallization at higher transition temperatures. Under constant stress, the pre-alignment promotes crystal growth along the mechanically induced director resulting in a substantial increase of deformation in favor of that direction. These results show how mechanical ensemble, deformation, and cross-linking can be combined to tailor the shape response of polymer networks upon phase transition.

CPP 59.6 Fri 12:45 ZEU/0260

Surface-induced ordering and continuous breaking of translational symmetry in conjugated polymers — Anton Sinner, Alexander Much, and •Oleksandr Dolynchuk — Martin Luther University Halle-Wittenberg, Germany

Surface-induced liquid crystalline (LC) phase transitions elicit fundamental interest and hold potential for leveraging the accompanying anisotropic order at the surface. Board-like conjugated polymers are of particular interest due to the novel sanidic LC phases they exhibit, which have remained largely unexplored. Specifically, although preferential molecular orientation near the free surface has been observed in films of conjugated polymers, the mechanism of its formation is not yet fully understood. In this study, grazing-incidence X-ray scattering is employed to monitor the formation and breaking of positional order in situ in thin films of two conjugated polymers representative of two classes: polythiophenes and polydiketopyrrolopyrroles. Our findings demonstrate that the surface induces positional order in films of both conjugated polymers via the formation of a highly oriented, sanidic disordered LC phase. The ordering process continues upon cooling and undergoes multiple LC transitions into more ordered phases, both at the surface and in the bulk, which can compete with each other. The positional smectic-like order parameter displays continuous temperature dependence in the vicinity of the transition, signifying a continuous breaking of translational symmetry by the surface. Theoretical analysis enables accurate description of the order parameter when critical behavior is considered.

CPP 60: Molecular and Polymer Dynamics, Friction and Rheology II

Time: Friday 12:15–13:00 Location: HÜL/S386

CPP 60.1 Fri 12:15 HÜL/S386

Fouling in Emulsion Polymerization of Different Copolymers investigated in-situ with the Quartz Crystal Microbalance (QCM) — •Kevin Marvin Hoffmann and Diethelm Johannsmann — Clausthal University of Technology, Institute of Physical Chemistry, Arnold-Sommerfeld-Straße 4, 38678 Clausthal-Zellerfeld, Germany

In emulsion polymerization, reaction and particulate fouling leads to clogging, product contamination, and reduced heat transfer efficiency. Common techniques for in-line monitoring of fouling are based on the heat transfer efficiency across the surface and the pressure drop in pipes or tubes. These techniques show fouling layers at thicknesses of a few tens of micrometers, at least. They are not sensitive enough to study the initial stages of a fouling.

A quartz crystal microbalance with dissipation monitoring (QCM-D) was used to study fouling in-situ. The QCM infers changes in mass on its surface to changes of its resonance frequency. It is sensitive down to the nanometer range. In addition to an estimate of the layer thickness, the QCM-D provides for additional information, derived from the comparison between the shifts in frequency and half-bandwidth as well as the comparison between different overtones.

It was found that polyacrylates behaved characteristically differently from polyvinyl acetates. The polyacrylates formed compact and stiff fouling layers. The polyvinyl acetates formed softer and more porous, extended layers. We assume that the stabilizing agent has a major impact on the fouling layer's nature.

CPP 60.2 Fri 12:30 HÜL/S386

Cluster growth dynamics of nickel particles in viscoelastic matrices — •Konstantin Gerstenberger und Günter K. Auernhammer — Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, 01069 Dresden, Germany

Magnetic elastomers can dynamically modify their mechanical properties in response to a magnetic field giving them the potential for new applications as soft actuators. A common method of producing these materials involves embedding magnetic particles in an elastomer matrix. In the presence of an applied magnetic field, the particles tend to arrange themselves into chain-like clusters which react to external stimuli, even if the matrix is crosslinked.

As part of the research unit FOR 5599 on structured magnetic elastomers we investigate the formation process of these materials, paying particular attention to the interaction between particle cluster formation and simultaneous cross-linking of the surrounding matrix. We use particle tracking velocimetry techniques to observe the cluster development over time and investigate how this process depends on various parameters. Therefore, it can be concluded that the development of chains is influenced by not only the particle concentration and matrix viscosity, but also the rotation of the applied magnetic field. This rotation can be used to adjust the mean length of the chains to a specific value.

Further investigation of larger sample sizes will be possible due to a new kind of Hallbach array that is currently under construction. This presentation will also cover the general idea of this machine.

CPP 60.3 Fri 12:45 HÜL/S386

Maps of High Viscoelastic Properties Generated with an Instrument Combining a Quartz Crystal Microbalance (QCM) with an AFM — •Cedric Jünemann, Diethelm Johannsmann, and Arne Langhoff — Clausthal University of Technology, Instutite of Physical Chemistry, Arnold-Sommerfeld-Straße 4, 38678 Clausthal-Zellerfeld

We present an instrument, which images the high-frequency viscoelastic properties of various samples. The instrument combines an atomic force microscope (AFM) with a quartz crystal microbalance with dissipation monitoring (QCM-D). Imaging becomes possible by a fast measurement of a resonator's frequency and bandwidth, achieved with a multi-frequency lockin amplifier (MLA). The MLA tracks multiple overtones simultaneously. To improve contrast and to facilitate quantitative interpretation, the colloidal force probe configuration was used. The cantilever was modified by gluing a glass sphere with a diameter of 50 μm to the tip, thereby increasing the contact radius to a few hundred nanometers. The sphere is heavy enough to clamped in place by inertia, which simplifies the analysis. A quantitative interpretation can rely on ratios between the different QCM signals, which eliminates the unknown contact area from the analysis. Printed drops and a biofilm composed of yeast were chosen for demonstration. This approach provides for a flexible method to investigate viscoelastic properties on the nanoscale at high frequencies.

CPP 61: Closing Talk (joint session CPP/BP/DY)

Time: Friday 13:15–14:00 Location: HSZ/0002

Invited Talk CPP 61.1 Fri 13:15 HSZ/0002

Biomolecular Condensates: Challenges for Polymer Physics

— •Jens-Uwe Sommer — Leibniz-Insitut für Polymerforschung Dresden, Bereich Theorie der Polymere,Hohe Straße 6, 01069 Dresden, Germany — TU Dresden, Insitut für Theoretische Physik, Zellescher Weg 17, D-01069 Dresden, Germany

Biomolecular condensates (BMCs) constitute an emerging paradigm in the understanding of biological functions. They shift the focus from individual biochemical processes toward the collective behavior of biopolymers, in which phase-separation mechanisms and intrinsically disordered proteins lacking canonical enzymatic roles play central and often decisive functions. Consequently, universal principles of complex (bio)polymer solutions gain relevance, and several classical questions in the physics of living matter can now be revisited from this polymer-physics perspective. In this talk, I will discuss theoretical approaches and concepts that are based on universal principles, with a particular emphasis on current challenges in the field.