Biological Physics Division
Fachverband Biologische Physik (BP)

Kerstin Blank
Institut für Experimentalphysik
Johannes Kepler Universität Linz
Altenberger Straße 69
4040 Linz, Österreich
kerstin.blank@jku.at

Kristian Franze
Institut für Medizinische Physik und Mikrogewebetechnik
Friedrich-Alexander-Universität Erlangen und Max-Planck-Zentrum für Physik und Medizin
Kussmaulallee 2
91054 Erlangen
kristian.franze@fau.de

Stefan Klumpp
Institut für Dynamik komplexer Systeme
Universität Göttingen
Friedrich-Hund-Platz 1
37077 Göttingen
stefan.klumpp@uni-goettingen.de

Overview of Invited Talks and Sessions

(Lecture halls H44 and H46; Poster P3 and P4)

Invited Talks

BP 3.7	Mon	11:15–11:45	H44	**Killing to survive - how protein-lipid interactions drive programmed cell death** — •Kristyna Pluhackova
BP 4.1	Mon	9:30–10:00	H46	**Spatiotemporal organization of bacterial biofilm formation and functions** — •Knut Drescher
BP 7.1	Mon	15:00–15:30	H44	**Single-molecule dynamic structural biology with Graphene Energy Transfer** — •Philip Tinnefeld, Alan Szalai, Giovanni Ferrari, Lars Richter, Ingrid Tessmer, Andres Vera-Gomez, Izabela Kaminska
BP 8.6	Mon	16:15–16:45	H46	**In situ control of cells and multicellular structures at the microscale by two-photon lithography** — •Christine Selhuber-Unkel
BP 11.1	Tue	9:30–10:00	H44	**Network connectivity determines the mechanisms responsible for cytoskeletal elasticity** — •Martin Lenz
BP 15.1	Tue	11:45–12:15	H44	**Does Oncology Need Physics of Cancer?** — •Josef Käs
BP 18.1	Wed	9:30–10:00	H44	**Mechanical Imprints of Cell Competition** — •Benoit Ladoux
BP 19.8	Wed	11:30–12:00	H46	**Rolling vesicles: From confined rotational flows to surface-enabled motion** — •Laura R. Arriaga, Paula Magrinya, Pablo Palacios, Pablo Llombart, Rafael Delgado-Buscalioni, Alfredo Alexander-Katz, Juan L. Aragones
BP 20.6	Wed	16:30–17:00	H44	**Centrosome positioning in cell migration and immune response** — •Heiko Rieger
BP 22.1	Wed	15:00–15:30	H46	**From DNA Nanotechnology to biomedical insight: Towards single-molecule spatial omics** — •Ralf Jungmann
BP 25.1	Thu	9:30–10:00	H44	**Oncogenic signaling and stiffness sensing** — •Johanna Ivaska
BP 26.6	Thu	11:00–11:30	H46	**Theory for sequence selection via phase separation and oligomerization** — •Christoph Weber
BP 29.1	Thu	15:00–15:30	H44	**Community-driven software and data training for computational biology** — •Toby Hodges
BP 30.5	Thu	16:00–16:30	H46	**Topology in biological matter - are there double knots in proteins or maybe even more complicated knots? Prediction and in vitro verification.** — •Joanna I Sulkowska
BP 31.1	Fri	9:30–10:00	H44	**Wave propagation in systems of active filaments** — •Kirsty Y. Wan
BP 35.1	Fri	13:15–14:00	H2	**Active control of forces, movement and shape: from biological to non-living systems** — •Ulrich S. Schwarz

Invited Talks of the joint Symposium Physics of Embryonic Development Across Scales: From DNA to Organisms (SYED)

See SYED for the full program of the symposium.

SYED 1.1	Mon	9:30–10:00	H1	**Emergent crystalline order in a developing epithelium** — Kartik Chhajed, Natalie Dye, Marko Popović, •Frank Jülicher

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

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

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

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

See SYAI for the full program of the symposium.

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

Invited Talks of the joint Symposium Nonequilibrium Collective Behavior in Open Classical and Quantum Systems (SYQS)

See SYQS for the full program of the symposium.

SYQS 1.1	Thu	15:00–15:30	H1	**Active quantum flocks** — Reyhaneh Khasseh, Sascha Wald, Roderich Moessner, Christoph Weber, •Markus Heyl
SYQS 1.2	Thu	15:30–16:00	H1	**Robust dynamics and function in stochastic topological systems** — •Evelyn Tang
SYQS 1.3	Thu	16:00–16:30	H1	**Nonequilibrium Dynamics of Disorder-Driven Ultracold Fermi Gases** — •Artur Widera
SYQS 1.4	Thu	16:45–17:15	H1	**Topological classification of driven-dissipative nonlinear systems** — •Oded Zilberberg, Greta Villa, Kilian Seibold, Vincent Dumont, Gianluca Rastelli, Mateusz Michałek, Alexander Eichler, Javier del Pino
SYQS 1.5	Thu	17:15–17:45	H1	**Learning dynamical behaviors in physical systems** — •Vincenzo Vitelli

Sessions

BP 1.1–1.3	Sun	16:00–18:15	H2	**Hands-on Tutorial: AI Fundamentals for Research (joint session BP/TUT/DY/AKPIK)**
BP 2.1–2.11	Mon	9:30–12:45	H37	**Active Matter I (joint session DY/BP/CPP)**

BP 3.1–3.12	Mon	9:30–13:00	H44	**Computational Biophysics I**
BP 4.1–4.6	Mon	9:30–11:15	H46	**Bacterial Biophysics**
BP 5.1–5.6	Mon	11:30–13:00	H46	**Membranes and Vesicles I**
BP 6.1–6.7	Mon	15:00–17:00	H37	**Active Matter II (joint session BP/CPP/DY)**
BP 7.1–7.6	Mon	15:00–17:00	H44	**Single Molecule Biophysics**
BP 8.1–8.6	Mon	15:00–16:45	H46	**Biomaterials, Biopolymers and Bioinspired Functional Materials I (joint session BP/CPP)**
BP 9.1–9.4	Mon	17:00–18:00	H46	**Biomaterials, Biopolymers and Bioinspired Functional Materials II (joint session CPP/BP)**
BP 10.1–10.9	Tue	9:30–12:30	H43	**Focus Session: Nonlinear Dynamics in Biological Systems I (joint session DY/BP)**
BP 11.1–11.7	Tue	9:30–11:30	H44	**Cytoskeleton**
BP 12.1–12.6	Tue	9:30–11:15	H46	**Biomaterials, Biopolymers and Bioinspired Functional Materials III (joint session CPP/BP)**
BP 13.1–13.11	Tue	9:30–13:00	H47	**Active Matter III (joint session DY/BP/CPP)**
BP 14.1–14.25	Tue	10:00–12:30	P3	**Poster Session I**
BP 15.1–15.4	Tue	11:45–13:00	H44	**Cell Mechanics I**
BP 16.1–16.4	Tue	14:00–15:15	H43	**Focus Session: Nonlinear Dynamics in Biological Systems II (joint session DY/BP)**
BP 17.1–17.82	Tue	18:00–20:30	P4	**Poster Session II**
BP 18.1–18.12	Wed	9:30–13:00	H44	**Tissue Mechanics**
BP 19.1–19.12	Wed	9:30–13:00	H46	**Membranes and Vesicles II**
BP 20.1–20.10	Wed	15:00–18:00	H44	**Statistical Physics of Biological Systems I (joint session BP/DY)**
BP 21.1–21.9	Wed	15:00–17:30	H45	**Networks, From Topology to Dynamics (joint session SOE/BP/DY)**
BP 22.1–22.9	Wed	15:00–17:45	H46	**Bioimaging**
BP 23.1–23.1	Wed	18:00–20:00	P2	**Poster Focus Session Chemical Imaging for the Elucidation of Molecular Structure (joint session O/BP)**
BP 24	Wed	18:15–19:15	H46	**Members' Assembly**
BP 25.1–25.12	Thu	9:30–13:00	H44	**Cell Mechanics II**
BP 26.1–26.9	Thu	9:30–12:15	H46	**Synthetic life-like systems and Origins of Life**
BP 27.1–27.7	Thu	15:00–17:30	H24	**Focus Session Chemical Imaging for the Elucidation of Molecular Structure I (joint session O/BP)**
BP 28.1–28.9	Thu	15:00–17:45	H37	**Microswimmers and Microfluidics (joint session DY/BP/CPP)**
BP 29.1–29.11	Thu	15:00–18:00	H44	**Focus Session: Innovations in Research Software Engineering (joint session BP/DY)**
BP 30.1–30.10	Thu	15:00–18:00	H46	**Protein Structure and Dynamics**
BP 31.1–31.12	Fri	9:30–13:00	H44	**Active Matter IV (joint session BP/CPP/DY)**
BP 32.1–32.13	Fri	9:30–13:00	H46	**Computational Biophysics II**
BP 33.1–33.7	Fri	10:30–12:45	H24	**Focus Session Chemical Imaging for the Elucidation of Molecular Structure II (joint session O/BP)**
BP 34.1–34.5	Fri	11:30–13:00	H43	**Statistical Physics in Biological Systems II (joint session DY/BP)**
BP 35.1–35.1	Fri	13:15–14:00	H2	**Closing Talk (joint session BP/CPP/DY)**

Members' Assembly of the Biological Physics Division

Wednesday 18:15–19:15 H46

- Report of the speaker team
- Election of a new member of the speaker team
- Any other business

BP 1: Hands-on Tutorial: AI Fundamentals for Research (joint session BP/TUT/DY/AKPIK)

Artificial intelligence (AI) has become an essential tool in modern physics, enabling new approaches to data analysis, modeling, and prediction. This hands-on tutorial provides an accessible introduction to key AI concepts, emphasizing their practical applications in physics research.

Please bring your laptop. There will be limited power outlets in the room, so come with a fully charged battery.

Materials will be made available from 10.03.2025, accessible via the following options:
GitHub repository:
https://github.com/RedMechanism/DPG-SKM-2025-Tutorial-AI-Fundamentals-for-Research
ZIP file download:
https://jlubox.uni-giessen.de/getlink/fiAGRzcGTiCL3GZxk8WAjom4/
Participants are encouraged to download them ahead of time.

Organized by Jan Bürger (Aachen), Janine Graser (Duisburg), Robin Msiska (Duisburg/Ghent), and Arash Rahimi-Iman (Gießen), with support from Stefan Klumpp (Göttingen) and Tim Ruhe (Dortmund).

Time: Sunday 16:00–18:15 Location: H2

Tutorial BP 1.1 Sun 16:00 H2
Introduction — Jan Bürger[1], •Janine Graser[2], Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

The session begins with an overview of essential AI concepts, including neural networks, training methodologies, and key distinctions between AI models. Participants will gain a foundational understanding of AI principles and how these tools can be leveraged for various research challenges.

5 min. break

Tutorial BP 1.2 Sun 16:40 H2
Hands-On Session 1 – Function Approximation — •Jan Bürger[1], Janine Graser[2], Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

In the first half of the interactive session, participants will work with Jupyter Notebooks to explore practical applications of machine learning. They will train simple neural networks to predict a mathematical function, gaining hands-on experience in tuning key parameters. Since neural networks can typically be considered universal function approximators, this concept is effectively illustrated using a one-dimensional function, making it easy to visualize and understand.

5 min. break

Tutorial BP 1.3 Sun 17:30 H2
Hands-On Session 2 – Classification and More — Jan Bürger[1], Janine Graser[2], •Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

The session demonstrates how pre-trained models can simplify tasks such as classification, making them readily applicable to research. Typical examples include recognizing handwritten digits, which showcase the power of pretrained models in solving common challenges. As a preview of advanced topics, the tutorial concludes with brief examples of large language models (LLMs) and generative AI.

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

Time: Monday 9:30–12:45 Location: H37

BP 2.1 Mon 9:30 H37
Odd dynamics and pattern formation in mixtures of magnetic spinners and passive colloids — •Dennis Schorn[1], Stijn van der Ham[2], Hanumantha Rao Vutukuri[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, 64289 Darmstadt, Germany — [2]MESA+ Institute, University of Twente, 7500 AE Enschede, The Netherlands

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

BP 2.2 Mon 9:45 H37
Symmetry breaking in active non-reciprocal systems — •Kim L. Kreienkamp and Sabine H. L. Klapp — TU Berlin, Germany

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

Our simulations confirm that spontaneous chirality arises at the particle level. In particular, we observe chimera-like states with coexisting locally synchronized and disordered regions. At the coupling strengths associated with exceptional points, the spontaneous chirality peaks.

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

BP 2.3 Mon 10:00 H37

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

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

BP 2.4 Mon 10:15 H37

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

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

BP 2.5 Mon 10:30 H37

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

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

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

Invited Talk BP 2.6 Mon 10:45 H37

Collective behavior of photoactive macroscopic particles — •Iker Zuriguel — University of Navarra, Pamplona, Spain

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

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

15 min. break

BP 2.7 Mon 11:30 H37

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

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

BP 2.8 Mon 11:45 H37

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

Swarmalators are an active matter system of oscillators which exhibit swarming and collective motion in physical space, as well as synchronization behavior in an additional phase variable space, originally introduced by O'Keeffe *et al.* (*Nat. Commun.* 8(1), 1504, 2017). Such systems with bidirectional couplings in space and phase can be observed in nature, such as in the chorusing behavior of Japanese tree frogs characterized by Aihara *et al.* (*Sci. Rep.* 4(1), 3891, 2014). The interplay between attraction, repulsion, and phase synchronization provides several distinct regimes of self-organizational behavior.

Akin to biological swarm systems responding to predator interactions, swarmalators can respond collectively to external perturbations by a repulsive driver. In previous work, driving was realized with a mobile 'pacemaker' by Xu *et al.* (*Chaos* 34(11), 113103, 2024). The present study introduces a new 'predator-prey' driven swarmalator model showing rich adaptive behavior. This could have a wide variety of potential future applications, from biological physics to swarm robotics to nature-inspired learning algorithms and methods of inference.

BP 2.9 Mon 12:00 H37

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

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

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

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

BP 2.10 Mon 12:15 H37

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

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

BP 2.11 Mon 12:30 H37

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

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

BP 3: Computational Biophysics I

Time: Monday 9:30–13:00 Location: H44

BP 3.1 Mon 9:30 H44

RNA plasticity emerges as an evolutionary response to fluctuating environments — •Paula García-Galindo[1] and Sebastian E. Ahnert[1,2] — [1]Department of Chemical Engineering and Biotechnology, University of Cambridge, Philippa Fawcett Drive, Cambridge CB3 0AS United Kingdom — [2]The Alan Turing Institute, 96 Euston Road, London NW1 2DB, UK

Phenotypic plasticity, the ability of a single genotype to produce multiple distinct phenotypes, can be studied effectively using RNA. RNA is a dynamic macromolecule that probabilistically shifts its structure due to thermal fluctuations at the molecular scale. To model the evolution of RNA plasticity, we use the RNA sequence-to-structure non-deterministic mapping, a computationally tractable genotype-phenotype (GP) map where probabilistic phenotypes are derived from the Boltzmann distribution of structures for each RNA sequence. Through evolutionary simulations with periodic environmental switching on the GP map, we observe that RNA phenotypes adapt to these fluctuations by evolving toward optimal plasticity. These optimal phenotypes are defined by nearly equal Boltzmann probabilities for distinct structures, each representing the most advantageous configuration for alternating environments. Our findings demonstrate that phenotypic plasticity, a widespread biological phenomenon, is a fundamental evolutionary adaptation to fluctuating environments.

BP 3.2 Mon 9:45 H44

Symmetry of loop extrusion by dimeric SMC complexes is DNA-tension-dependent — Biswajit Pradhan[1], •Adrian John Pinto[2], Peter Virnau[2], and Eugene Kim[1] — [1]Max Planck Institute of Biophysics, 60438 Frankfurt am Main, Germany — [2]Institut für Physik, Staudingerweg 9, Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany

Structural maintenance of chromosome (SMC) complexes are involved in genome organization and regulation via DNA loop extrusion. During extrusion SMC proteins reel DNA from one or both sides and a loop forms and increases. At low DNA tension (< 0.1pN), Smc5/6 and Wadjet extrude DNA from both sides of the loop. At higher tension, however, they transition to a behavior akin to one-sided extruders, yet still capable of extruding from one or the other side thereby switching the direction of extrusion [1]. In order to model this process in simulations, we propose a coarse-grained model for DNA loop extrusion using a Kratky-Porod chain as a basis for DNA and a handcuff for SMC proteins. By matching stalling forces, we are able to simulate loop extrusion on experimental time and length scales. We find that the observed switching from two- to one-sided behavior does not require a change in motor activity, but can be explained as a complex interplay of extrusion, stalling and thermal fluctuations.

[1] Pradhan, B., Pinto, A., Kanno, T., et al. (2024). Symmetry of loop extrusion by dimeric SMC complexes is DNA-tension-dependent. bioRxiv. https://doi.org/10.1101/2024.09.12.612694

BP 3.3 Mon 10:00 H44

NucleoSeeker - Precision filtering of RNA databases to curate high-quality datasets — •Utkarsh Upadhyay[1], Fabrizio Pucci[2], Julian Herold[3], and Alexander Schug[1,4] — [1]Jülich Supercomputing Centre, Germany — [2]Universite Libre de Bruxelles, Belgium — [3]Karlsruhe Institute for Technology, Germany — [4]University of Duisburg- Essen, Germany

The structural prediction of biomolecules via computational methods complements the often involved wet-lab experiments. Unlike protein structure prediction, RNA structure prediction remains a significant

challenge in bioinformatics, primarily due to the scarcity of RNA structure data and its varying quality. Many methods have used this limited data to train deep learning models but redundancy, data leakage and bad data quality hampers their performance. In this work, we present NucleoSeeker, a tool designed to curate high-quality, tailored datasets from the Protein Data Bank (PDB) database. It is a unified framework that combines multiple tools and streamlines an otherwise complicated process of data curation. It offers multiple filters at structure, sequence and annotation levels, giving researchers full control over data curation. Further, we present several use cases. In particular, we demonstrate how NucleoSeeker allows the creation of a non-redundant RNA structure dataset to assess AlphaFold3's performance for RNA structure prediction. This demonstrates NucleoSeeker's effectiveness in curating valuable non-redundant tailored datasets to both train novel and judge existing methods. NucleoSeeker is very easy to use, highly flexible and can significantly increase the quality of RNA structure datasets.

BP 3.4 Mon 10:15 H44

Uncovering the Non-Canonical RNA Binding site on the Immune Sensor OAS2 by combining AI, MD simulations and experiments. — •Adrian F. Schnell[1], Veronika Merold[2], Indra Bekere[2], Carina C. de Oliveira Mann[2], and Nadine Schwierz[1] — [1]Institute of Physics, University of Augsburg — [2]Department of Bioscience, Technical University of Munich

Molecular dynamics (MD) simulations and machine learning provide powerful tools to predict protein-RNA interactions, but their predictions require experimental verification. In this talk, we showcase an advancement in understanding the immune sensor 2'-5'-oligoadenylate synthetase 2 (OAS2) by combining AlphaFold 3, MD simulations, cryo-electron microscopy (cryo-EM), and cellular assays. Although the structure of the OAS2 has been resolved through cryo-EM, the precise mechanisms underlying its activation and the RNA binding site remained elusive.

To fill this gap, we combined all-atom MD simulations based on cryo-EM structures and AlphaFold 3 predictions to identify non-canonical RNA binding interfaces on the catalytically deficient OAS2 domain. By integrating mutagenesis studies and contact data from MD simulations, we uncovered critical structural details of RNA binding and OAS2 activation. Importantly, our findings reveal how OAS2 domains discriminate RNA length, providing new insights into its function and regulatory mechanisms. These results enhance our understanding of OAS2's antiviral immune role and offer a foundation for developing antiviral strategies targeting the OAS-RNase L pathway.

BP 3.5 Mon 10:30 H44

Computational bridging between sequence design and network-level behaviour of programmable DNA-nanomotifs — •Aaron Gadzekpo[1] and Lennart Hilbert[1,2] — [1]Karlsruhe Institute of Technology, Institute of Biological and Chemical Systems — [2]Karlsruhe Institute of Technology, Zoological Institute

DNA can serve as a programmable material, by using the DNA sequence to control the 3D-structure of building blocks at the nanometre-scale. In our work, we construct X-shaped particles, or "nanomotifs", from four single-stranded DNA-oligomers, each 46 nucleotides in length. The X-motifs' four arms selectively and transiently hybridize, linking into large, dynamic networks guided by DNA sequence complementarity. We present our scale-bridging computational methods to predict how DNA-oligomer sequences translate into physical properties of X-motifs and the emergent behaviour of networks. In particular, we leverage machine learning to transition from base-pair resolution simulations of single X-motifs and linked pairs to coarse-grained molecular dynamics simulations of networks at increased time and length scales. These simulations are used to explore how nanomotif design at nucleotide level influences emergent behaviour, including liquid-liquid phase separation and condensation on target DNA strands with complementary binding motifs. We connect our observation to corresponding experiments, showcasing model-aided design of DNA-based materials.

BP 3.6 Mon 10:45 H44

Ionizable cationic lipids and helper lipids synergistically contribute to RNA packing and protection in lipid-based nanomaterials — •David Noel Zimmer[1,2], Friederike Schmid[1], and Giovanni Settanni[1,2] — [1]Physics Department Johannes Gutenberg University Mainz — [2]Faculty of Physics and Astronomy Ruhr University Bochum

Lipid-based nanomaterials are used as a common delivery vehicle for RNA therapeutics. They typically include a formulation containing ionizable cationic lipids, cholesterol, phospholipids, and a small molar fraction of PEGylated lipids. The ionizable cationic lipids are considered a crucial element of the formulation for the way they mediate interactions with the anionic RNA as a function of pH. Here[1], we show, by means of molecular dynamics simulation of lipid formulations containing two different ionizable cationic lipids (DLinDMA and DLinDAP), that the direct interactions of those lipids with RNA, taken alone, may not be sufficient to determine the level of protection and packaging of mRNA. Our simulations help and highlight how the collective behavior of the lipids in the formulation, which determines the ability to envelop the RNA, and the level of hydration of the lipid-RNA interface may also play a significant role. This allows the drawing of a hypothesis about the experimentally observed differences in the transfection efficiency of the two ionizable cationic lipids.

[1] Zimmer, D. N., Schmid, F., & Settanni, G. (2024). J. Phys. Chem. B 2024, 128, 41, 10165-10177.

15 min. break

Invited Talk BP 3.7 Mon 11:15 H44

Killing to survive - how protein-lipid interactions drive programmed cell death — •Kristyna Pluhackova — University of Stuttgart, Stuttgart, Germany

Programmed cell death is an essential process of eukaryotic life, enabling e.g., embryonic development, regeneration, or fighting pathogens. Depending on the needs of an organism, diverse molecular mechanisms of cell death exist, determining among others the speed of cell death, its extent and the impact on surrounding cells. Not surprisingly, dysregulation of cell death culminates in diverse diseases, the most prominent of all being cancer.

Here, I reveal molecular details of protein-lipid interactions in programmed cell death by multiscaling molecular dynamics simulations. First, I unveil how lipids unplug medium-sized membrane pores formed by a pyroptotic agent gasdermin and reveal astonishing adaptability of the pore shape. Next, I demonstrate how the gasdermin species and the lipid composition determine the process of gasdermin pore formation. At last, I resolve the mechanism through which ninjurin-1 disrupts membranes during plasma membrane rupture, the terminal event of many cell-death processes.

BP 3.8 Mon 11:45 H44

Integrative Modeling of Cellular Dynamics: Applications to Viruses and Neurotransmission — •Mohsen Sadeghi — Freie Universität Berlin, Berlin, Germany

A comprehensive understanding of cellular processes requires a quantitative analysis of biomembrane dynamics in interaction with protein populations, within a model that integrates kinetics and protein structural information. This is crucial for deciphering and potentially manipulating complex biological pathways. In this work, we introduce a dynamic framework for modeling membranes and proteins [1-5], showcasing its large-scale applications. These include the first computational model of the human cytomegalovirus [6] and the simulation of synaptic vesicle docking. We highlight how large-scale mesoscopic simulations provide unprecedented insights into complex cellular dynamics, capturing spatiotemporal scales that are directly relevant to cell biology.

1 Sadeghi and Noé, Nat. Commun. (2020) 11:2951.

2 Sadeghi, Weikl and Noé, J. Chem. Phys. (2018) 148:044901.

3 Sadeghi and Noé, J. Chem. Phys. (2021) 155:114108.

4 Sadeghi and Noé, J. Phys. Chem. Lett. (2021) 12:10497-10504.

5 Sadeghi, Soft Matter (2022) 18:3917-3927.

6 Bogdanow, et al. Nat. Microbiol. (2023) 8:1732.

BP 3.9 Mon 12:00 H44

Hepatitis C Virus Infection Alters NK Cell Receptor Expression: A High-Dimensional Analysis — •Andrea Schneider — Heirich-Heine Universität Düsseldorf

Hepatitis C virus (HCV) infection influences the expression of receptors on natural killer (NK) cells, a crucial component of the innate immune system. Using fluorescent markers for flow cytometry measurements, receptor expression can be analyzed to identify differences between healthy individuals, recovered patients, and those with chronic infections. Due to the possibility of using many markers simultaneously in

one measurement, algorithms for dimension reduction are necessary for the evaluation of flow cytometry data. These findings could provide a potential starting point for novel therapeutic approaches. A key focus of the talk is the application of t-SNE, a dimensionality reduction algorithm that visualizes high-dimensional data in two-dimensional scatterplots while preserving high-dimensional clustering. The analysis offers valuable insights into the cellular differences among the three patient groups and opens new perspectives for immunological research.

BP 3.10 Mon 12:15 H44

Activity enhanced shear-thinning of flexible linear polar polymers — •Arindam Panda[1], Roland G. Winkler[2], and Sunil P Singh[1] — [1]Indian Institute Of Science Education and Research, Bhopal, Madhya Pradesh, India — [2]Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany

The rheological behavior of tangentially propelled flexible polymers in linear shear flow is investigated through computer simulations and compared with analytical predictions. Our study reveals a significant interplay between nonequilibrium active forces and shear-induced effects on the polymer's structural and dynamical properties. Polar activity enhances the shear-induced stretching along the flow direction while inducing compression in the transverse direction. This coupling leads to a pronounced shear-thinning response, where the viscosity decreases with increasing shear rate. In the high activity and shear limit, the polymer's behavior becomes largely independent of the active forces, with the shear flow predominantly driving the system's response. At asymptotically high shear rates, the system transitions to a regime where the polymer exhibits characteristics akin to passive polymers, with shear forces entirely overshadowing the influence of activity.

BP 3.11 Mon 12:30 H44

Patchy Particle Model for Biomolecular Condensates — •Devika Magan[1,2,3], Alena Taskina[1,4], Simon Dannenberg[1], and Stefan Klumpp[1,4] — [1]Institute for the Dynamics of Complex Systems, University of Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen, Germany — [2]Indian Institute of Science Education and Research Mohali, India — [3]Institute for Theoretical Physics, Heidelberg University, 69120 Heidelberg, Germany — [4]Max Planck School Matter to Life

Biomolecular condensates are formed via liquid-liquid phase separation (LLPS) of proteins and nucleic acids, driven by interactions between low-affinity binding sites. Computational studies of biomolecular condensates often use coarse-grained patchy particle models, representing proteins with a repulsive core and directional attractive patches. However, these simulations are typically limited by slow dynamics and struggle to capture the full range of material properties of fluid-like condensates. We present an enhanced patchy particle model to study the formation and dynamics of biomolecular condensates. By incorporating flexible patches and weak isotropic attractions between cores, our model preserves key equilibrium characteristics, including phase behavior and local structure, while significantly accelerating system dynamics. These modifications enable the simulation of larger, more complex systems previously inaccessible due to prohibitive relaxation times and provide a versatile tool for studying condensate dynamics.

BP 3.12 Mon 12:45 H44

Co-translational (polysome-protein) condensation — •Zhouyi He, Jens-Uwe Sommer, and Tyler Harmon — Leibniz Institute of Polymer Research , 01069, Dresden, Germany

Biomolecular condensates are ubiquitous in cells and play crucial roles in cellular regulation. These condensates typically form via liquid-liquid phase separation, where protein-protein interactions are crucial. However, how condensates interact with protein translation machinery is poorly studied. During translation, multiple ribosomes are simultaneously translating each mRNA forming a poly-ribosome structure (polysome), which resembles beads packed on a string. On one end of the mRNA, the ribosomes have only extruded the start of the nascent protein, and on the other end the ribosomes have a nearly finished protein. Nascent proteins from translating polysomes can interact with the finished proteins that make up the condensate (co-translational condensation). Using coarse-grained simulations, we show that the architecture of encoded proteins determines whether the polysome is adsorbed to the condensate surface or remains in the cytoplasm. Furthermore, we employ a reaction-diffusion model to analyze the time scales relevant to this process. Additionally, we model the potential cellular advantages of this phenomenon, including enhanced cellular response times, reduced noise in protein concentration, and facilitation of post-translational modifications. This work establishes a theoretical framework for co-translational condensation and highlights new functions for condensates in cells and offers promising directions for experimental validation.

BP 4: Bacterial Biophysics

Time: Monday 9:30–11:15 Location: H46

Invited Talk BP 4.1 Mon 9:30 H46

Spatiotemporal organization of bacterial biofilm formation and functions — •Knut Drescher — Biozentrum, University of Basel, Basel, Switzerland

In nature, bacteria often live in three-dimensional communities termed biofilms, in which cells are attached to each other through an extracellular matrix. In this presentation, I will first introduce microscopy, image processing, and spatiotemporal transcriptome measurement techniques that enable us to monitor all individual cells in living biofilms. Based on these techniques, I will then show how we can identify the cell-cell interaction processes that determine the architecture development of biofilm microcolonies, across different species. I will then proceed to discuss how individual cells in biofilms coordinate their activities so that the biofilm community develops emergent functions, such as the predation of human immune cells, as well as the protection from viral predators. This talk will therefore shed light on the spatiotemporal development of bacterial communities, and the mechanisms underlying emergent functions of these communities.

BP 4.2 Mon 10:00 H46

Modelling the growth of biofilms on soft substrates — •Anthony Pietz[1], Uwe Thiele[1], and Karin John[2] — [1]Universität Münster, Münster, Germany — [2]Université Grenoble Alpes

Bacteria invade surfaces by forming dense colonies encased in a polymer matrix. Successful settlement of founder bacteria, early microcolony development and later macroscopic spreading of these biofilms on surfaces rely on complex physical mechanisms. Data show that on soft hydrogels, substrate rigidity is an important determinant for biofilm initiation and spreading. Using a thermodynamically consistent thin-film approach for suspensions on soft elastic substrates we investigate in silico the role of substrate rigidity in the osmotic spreading of biofilms. We show that on soft substrates spreading is considerably slowed down and may even be arrested depending on the biomass production rate. We find, that the slowing down of biofilm spreading on soft surfaces is caused by a reduced osmotic influx of solvent into the biofilm results from the coupling between substrate deformation and interfacial forces.

BP 4.3 Mon 10:15 H46

Dynamics of bacterial growth and colony development in heterogeneous mechanical landscapes — •Chenyu Jin[1] and Anupam Sengupta[1,2] — [1]Physics of Living Matter Group, Department of Physics and Materials Science, University of Luxembourg, 162 A, Avenue de la Faïencerie, L-1511, Luxembourg — [2]Institute for Advanced Studies, University of Luxembourg, Avenue de l'Université, L-4365, Esch-sur-Alzette, Luxembourg

Bacteria inhabit diverse confinements, experiencing different mechanical cues including surface stiffness and adhesion, friction and wettability [1]. Recent studies have revealed how local crowding and phenotypic noise impact bacterial growth and structural changes like the monolayer-to-multilayer transitions (MTMT)[2,3]. Yet how colonies proliferate in heterogeneous physical landscapes remain largely unknown [4]. Here we combine quantitative imaging and numerical modeling to compare the dynamics of colony growth within soft hydrogels with those in liquid media for different bacterial species. We find that the growth rate typically decreases across species, at both the colony and individual scales, while the critical area at the MTMT increases

by an order of magnitude in the confined environment. An accompanying bioenergetic model offers mechanistic insights into the colony development in heterogeneous mechanical settings.

[1] NAM Araújo, LMC Janssen, et al., *Soft Matter* 19, 1695-1704 (2023). [2] R Wittmann, ..., A Sengupta, *Commun. Phys.* 6, 331 (2023). [3] J Dhar, ..., A Sengupta, *Nat. Phys.* 18, 945 (2022). [4] C Jin, A Sengupta, *Biophys. Rev.* 16, 2024

BP 4.4 Mon 10:30 H46

Capillary interactions organize bacterial colonies — •Ricard Alert[1,2,3], Matthew E. Black[4], Chenyi Fei[4,5], Ned S. Wingreen[4], and Joshua W. Shaevitz[4] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Center for Systems Biology Dresden — [3]Cluster of Excellence Physics of Life, TU Dresden — [4]Princeton University — [5]Massachusetts Institute of Technology

Many bacteria inhabit hydrated environments like soil, textiles and agar hydrogels in the lab. In these environments, cells are surrounded by a water meniscus, and they experience capillary forces. I will show that capillary forces organize bacterial colonies, enabling cells to aggregate into densely packed nematic layers while still allowing them to slide past one another. Our collaborators developed an experimental apparatus that allows us to control bacterial collective behaviors by varying the strength and range of capillary forces. Our results suggest that capillary forces may be a ubiquitous physical ingredient in shaping microbial communities in partially hydrated environments.

BP 4.5 Mon 10:45 H46

CISS Effect in Bacterial Extracellular Electron Transfer — •Nir Sukenik[1], Mohamad El Naggar[1], Yossi Paltiel[2], Ron Naaman[3], and Lech Tomasz Baczewski[4] — [1]University of Southern California, Lis Angeles, CA, USA — [2]Hebrew University of Jerusalem, Jerusalem, Israel — [3]Weizmann Institute of Technology, Rehovot, Israel — [4]Polish Academy of Sciences, Warsaw, Poland

Electron transfer through chiral molecules is characterized by a coupling between the electron velocity and its spin through the Chirality Induced Spin Selectivity (CISS) effect. Since most biomolecules are homochiral, it was recently hypothesized that CISS underlies the highly efficient electron transfer observed in biological systems by reducing the probability of electron backscattering. A remarkable example of efficient long-distance electron transport in biology is the extracellular respiration of metal-reducing bacteria, where a pathway composed of multiheme cytochromes facilitates extracellular electron transfer (EET) from the cellular interior to external electrodes. Using conductive probe atomic force microscopy measurements of protein monolayers adsorbed onto ferromagnetic substrates, we show that electron transport is spin selective in two of the multiheme cytochromes, the membrane-associated decaheme MtrA and the tetraheme periplasmic STC. To assess the in vivo physiological impact of CISS, we also present evidence that the respiration of a different EET capable bacterium, depends on the magnetization direction of the underlying ferromagnetic electrode. Taken collectively, our results demonstrate the important role of spin in a biological mechanism essential to life.

BP 4.6 Mon 11:00 H46

Slower prior growth in E. coli confers a competitive advantage under carbon starvation — •Zara Gough[1], Hamid Seyed Allaei[1], Severin Schink[2], Elena Biselli[1], Sophie Brameyer[3], and Ulrich Gerland[1] — [1]Physics of Complex Biosystems, Physics Department, Technical University of Munich, 85748 Garching, Germany — [2]Department of Systems Biology, Harvard Medical School, 200 Longwood Ave, Boston, MA 02115, USA — [3]Microbiology, Faculty of Biology, Ludwig Maximilians University Munich, Martinsried, Germany

Bacteria spend much of their life cycle under nutrient limitation, competing for resources to survive. Recent research has quantitatively characterized the carbon starvation kinetics of E. coli in monoculture using two experimentally measurable parameters: the maintenance rate and the recycling yield. Building on this framework, we show that these same parameters can predict fitness changes when cultures with distinct prior growth rates are subjected to starvation in co-culture. We introduce an additional model that explores the interaction between intracellular energy reserves and extracellular medium energy during co-culture starvation, and accounts for different uptake rates resulting from prior growth rate. Using a bottom-up approach to modelling that is derived directly from bacterial physiology, our work extends the quantitative understanding of population dynamics in E. coli.

BP 5: Membranes and Vesicles I

Time: Monday 11:30–13:00 Location: H46

BP 5.1 Mon 11:30 H46

In-Plane Correlations in Fluid Lipid Monolayers - Experiments and Molecular Dynamics Simulations — •Kay-Robert Dormann[1], Joshua Reed[1], Matej Kanduč[2], Benno Liebchen[1], and Emanuel Schneck[1] — [1]Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany — [2]Department of Theoretical Physics, Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia

Biological membranes predominantly consist of fluid lipid phases featuring lateral mobility and a considerable disorder of their hydrocarbon chains. Langmuir monolayers of lipids at the air/water interface are versatile model systems for fundamental physicochemical and biophysical membrane investigations. Recent experimental studies utilizing grazing-incidence x-ray diffraction (GIXD) have probed the chain correlation peak in fluid phospholipid monolayers as a function of the lipids' lateral packing. However, interpretation of the peak characteristics with over-simplified models based, for example, on rod-like chains yields only limited insights.

Here, we perform molecular dynamics (MD) simulations of phospholipids in the same monolayer configuration and predict the diffraction patterns originating from the chain correlations for a rigorous comparison with the experimental ones. The MD simulations reproduce the peak characteristics and their dependence on lateral packing well. Moreover, the experimentally validated simulation trajectories contain comprehensive information on the underlying chain correlations.

BP 5.2 Mon 11:45 H46

Modelling Wave Propagation on Monolayers — •Philipp Zolthoff and Jan Kierfeld — TU Dortmund, Dortmund, Germany

Recent experimental advances have enabled precise studies of pressure wave propagation through monolayers at the air-water interface, triggered by embedded azobenzenes and light-induced trans-to-cis isomerization. This talk presents theoretical results, which show that fractional nonlinear wave equations of Lucassen type can describe wave propagation on monolayers quantitatively. The nonlinear differential wave equation includes fractional time derivatives, incorporates measured Langmuir isotherms and a dynamic second viscosity that depends on the local state of the monolayer.

BP 5.3 Mon 12:00 H46

Artificial Membranes Through Physical Vapor Deposition (PVD): Exploring the Lipid Rafts Model — •Nancy Gómez-Vierling[1], D.A. Saavedra[1], M.A. Cisternas[2], M. Soto-Arriaza[3], C. Shen[4], P. Huber[4], and U.G. Volkmann[1] — [1]Instituto de Física, Pontificia Univ. Católica de Chile, Santiago, Chile — [2]Escuela de Ingeniería Industrial, Univ. de Valparaíso, Santiago, Chile — [3]Facultad de Medicina y Ciencia, Univ. San Sebastian, Santiago, Chile — [4]DESY, Hamburg, Germany

Essential to life, cell membranes are currently modelled as functional microdomains known as lipid rafts. These cholesterol- and sphingolipid-enriched domains are fundamental for organizing and categorizing key cellular processes. This research explores the assembly of artificial membranes inspired by the lipid raft model using PVD. This solvent-free technique previously demonstrated in DPPC membranes, is now applied to mixtures of sphingomyelin, cholesterol, and DOPC to investigate the self-assembly of microdomains under controlled conditions. Optimizing parameters such as temperature, deposition time, and thickness enables the successful formation of thin films on silicon substrates. Preliminary FTIR and GISAXS analyses confirm molecular integrity after cholesterol and DOPC evaporation, while ongoing studies examine the desorption and thermal stability of these SLBs.

This work advances our understanding of membrane physics and establishes a versatile platform for creating model membranes with potential applications in biotechnology and materials science. Acknowledgements: ANID Fellowships (DS, NGV); Puente UC 2024-25.

BP 5.4 Mon 12:15 H46

Structural and mechanical properties of lipid monolayers at the water-air interface — •Hyunyou Kim[1], Ivo Buttinoni[1], Laura Alvarez Frances[2], and Pantelis Mpourazanis[3] — [1]Institute of Experimental Physics of Condensed Matter, Heinrich-Heine University, Universitätsstr.1, 40225 Düsseldorf, Germany — [2]University of Bordeaux, CNRS, CRPP, UMR 5031, 33600 Pessac, France — [3]Fraunhofer IOSB, Gutleuthausstraße 1, 76275 Ettlingen, Germany

Lipid monolayers play a crucial role at air-water interfaces of body, such as in alveoli, where they regulate surface tension. When surface pressure increases, the interface transitions from liquid-expanded (LE) to liquid-condensed (LC) phases.

As experimental model, Dipalmitoylphosphatidylcholine (DPPC) and Cholesterol (Chol) are used. Langmuir-Blodgett trough monitors lipid monolayers during compression, while fluorescence microscopy visualizes the domains. Rheology is measured at various frequencies using an interfacial shear rheometer coupled with trough.

During compression, pure DPPC monolayers transition from LE to LC, with a plateau at surface pressure Π = 5-6 mN/m and collapse at Π = 60-65 mN/m. The domain shape changes from round to fractal. Adding Chol lowers the collapse pressure (Π = 45-50 mN/m) and eliminates the plateau when Chol exceeds 8.6 mol %. Rheology shows that Chol decreases surface viscosity and makes the monolayers more elastic at higher frequencies.

BP 5.5 Mon 12:30 H46

Study of Giant Unilamelar Vesicles' Fluidity in Microgravity Conditions — •Georgios Stogiannidis[1], Paulina Blair[1,3], Laura Alvarez[2], Thomas Voigtmann[1,3], and Ivo Buttinoni[1] — [1]Heinrich-Heine University, Düsseldorf, Germany — [2]Université de Bordeaux, Bordeaux, France — [3]Deutsche Zentrum für Luft- und Raumfahrt, Köln, Germany

In this study, we examine the effect of microgravity on the membrane fluidity of giant unilamellar vesicles (GUVs) made of DOPC and Cholesterol. GUVs are prepared using electroformation technique, during which a thin film of lipids is deposited on a conductive glass substrate while the application of AC electric field accelerates the swelling of the lipid film. We first study the fluidity of the vesicles over a range of DOPC/Cholesterol ratios using Fluorescence Recovery After Photobleaching (FRAP): a disk shaped area of the vesicle is bleached using a laser for a short amount of time and the fluidity is computed from the time of fluorescence-recovery time. The same fluidity also is investigated by means of fluorescence polarization anisotropy (FPA) technique, where the intensity of the sample's fluorescence emission is measured along two orthogonal polarization axes. The latter method can be implemented under microgravity conditions. We report a significant fluidity changes in microgravity conditions, where the vesicles display approximately 20% higher membrane fluidity compared to those measured on the ground. Our findings provide valuable insights on the cells' behavior in zero-gravity conditions and more specifically about the absorption of pharmaceuticals in the human body.

BP 5.6 Mon 12:45 H46

Translocation of vesicles through membrane-covered pores — •Nishant Baruah[1], Gerhard Gompper[1], Anil Kumar Dasanna[2], and Thorsten Auth[1] — [1]Theoretical Physics of Living Matter, Institute of Biological Information Processing and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Department of Physical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, Sector 81, Knowledge City, Mohali 140306, India

Apicomplexan parasites like Plasmodium, which transmits malaria, invade their host cells by translocating through a tight junction at the host plasma membrane. This process involves significant physical challenges, including the need for the parasite to deform its own membrane while squeezing through the tight junction and contending with the host membrane tension [1]. Here, we study as a model system the translocation of vesicles through membrane-covered pores driven by a contact interaction [2]. The calculations are performed using triangulated membranes and energy minimization. We predict stable translocation states for various vesicle- and host-membrane elastic properties and vesicle-to-pore size ratios. A finite-host membrane tension strongly suppresses pore translocation, which may explain protection against severe malaria in the Dantu blood group [3].

[1] S. Dasgupta et al, Biophys. J. 107, 43 (2014).
[2] N. Baruah et al. (https://doi.org/10.1101/2024.05.20.594296).
[3] S. N. Kariuki et al, Nature 585, 579 (2020).

BP 6: Active Matter II (joint session BP/CPP/DY)

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

BP 6.1 Mon 15:00 H37

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

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

BP 6.2 Mon 15:15 H37

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

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

BP 6.3 Mon 15:30 H37

Isovolumetric dividing active matter — Samantha R. Lish[1], Lukas Hupe[1], Ramin Golestanian[1,2], and •Philip Bittihn[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen,

Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

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

BP 6.4 Mon 15:45 H37

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

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

15 min. break

BP 6.5 Mon 16:15 H37

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

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

BP 6.6 Mon 16:30 H37

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

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

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

BP 6.7 Mon 16:45 H37

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

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

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

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

BP 7: Single Molecule Biophysics

Time: Monday 15:00–17:00 Location: H44

Invited Talk BP 7.1 Mon 15:00 H44

Single-molecule dynamic structural biology with Graphene Energy Transfer — •Philip Tinnefeld[1], Alan Szalai[1], Giovanni Ferrari[1], Lars Richter[1], Ingrid Tessmer[2], Andres Vera-Gomez[1], and Izabela Kaminska[1] — [1]Chemistry Department and Center for NanoScience, Ludwig-Maximilians-Universität München — [2]Rudolf Virchow Center, University of Würzburg, Würzburg

Obtaining structural information from single molecules is commonly associated with Fluorescence Resonance Energy Transfer that typically yields one distance between a fluorescent donor and an acceptor. Energy transfer to graphene with graphene-on-glass coverslips can extend the dynamic range to more than 30 nm. Based on the discovery that DNA can be placed vertically on graphene, we developed GETvNA (graphene energy transfer with vertical nucleic acids) that enables Angstrom precise visualization of DNA conformations and protein-DNA complexes. We envision that the alignment of DNA will additionally make it amenable to combined energy transfer and super-resolution interrogation for dynamic structural biology.

BP 7.2 Mon 15:30 H44

Doubling the resolution of fluorescence-lifetime single-molecule localization microscopy with image scanning microscopy — •Niels Radmacher[1], Oleksii Nevskyi[1], José Ignacio Gallea[1], Jan Christoph Thiele[2], Ingo Gregor[1], Silvio O. Rizzoli[3,4], and Jörg Enderlein[1,4] — [1]Third Institute of Physics, Georg August University, Göttingen, Germany — [2]Department of Chemistry, University of Oxford, Oxford, UK — [3]Department of Neuro- and Sensory Physiology, University Medical Center Göttingen, Göttingen, Germany — [4]Cluster of Excellence - Multiscale Bioimaging: from Molecular Machines to Networks of Excitable Cells (MBExC),Göttingen, Germany

In this study, we integrate a single-photon detector array into a confocal laser scanning microscope, enabling the combination of fluorescence-lifetime single-molecule localization microscopy with image scanning microscopy. This unique combination delivers a twofold improvement in lateral localization accuracy for single-molecule localization microscopy (SMLM) and maintains its simplicity. Moreover, the addition of lifetime information from our confocal laser scanning microscope eliminates chromatic aberration, particularly crucial for achieving few-nanometre resolution in SMLM. Our approach is named fluorescence-lifetime image scanning microscopy iSMLM. And is demonstrated through dSTORM and DNA PAINT experiments on fluorescently labelled cells, showcasing both resolution enhancement and fluorescence-lifetime multiplexing capabilities.

BP 7.3 Mon 15:45 H44

Two-color single-molecule coincidence detection for the analysis of biological processes and high-affinity bi-molecular binding — •Benno Schedler[1], Olessya Yuknovets[1], Alida Meyer[1], Lennart Lindner[1], and Jörg Fitter[1,2] — [1]RWTH Aachen University, I. Physikalisches Institut (IA), Aachen, Germany — [2]FZ Jülich, ER-C-3, Jülich, Germany

Life on the molecular scale is based on a versatile interplay of biomolecules, a feature that is relevant for the formation of macromolecular complexes. Fluorescence based two-color coincidence detection is widely used to characterize molecular binding and was recently improved by a brightness-gated version which gives more accurate results [1]. We developed and established protocols which make use of coincidence detection to quantify binding fractions between interaction partners labeled with fluorescence dyes of different colors. Since the applied technique is intrinsically related to single molecule detection, the concentration of diffusing molecules for confocal detection is typically in the low pico-molar regime. This makes the approach a powerful tool for determining bi-molecular binding affinities, in terms of KD-values, in this regime. By measuring the affinity at different temperatures, we were able to determine thermodynamic parameters of the binding interaction. The results show that the ultra-tight binding is dominated by entropic contributions [2].

References:

[1] Höfig et al. Communication Biology 2019 2, 459

[2] Schedler et.al. Int. J. Mol.Sci 2023 24, 16379

15 min. break

BP 7.4 Mon 16:15 H44

Maximizing Flavor: Leveraging Nano-biophysical Methods in Food Perception and Formulation Research — •Melanie Koehler — Leibniz-Institute for Food Systems Biology at the Technical University of Munich, Lise Meitner-Straße 34, 85354 Freising, Germany — TUM Junior Fellow at the Chair of Nutritional Systems Biology, Technical University of Munich, Lise-Meitner-Straße 34, 85354 Freising, Germany

The food industry faces the challenge of creating healthier products with less salt, sugar, fat, and calories while maintaining flavor and consumer satisfaction. Flavor perception, influenced by taste, smell, texture, and individual factors, requires a deeper understanding to drive innovation. This research highlights the use of nano-biophysical techniques, particularly bio atomic force microscopy (AFM), to explore taste and texture at the molecular level. AFM provides nanoscale insights into food components' interactions with sensory receptors (taste- and mechanoreceptors), and their role in flavor release. For instance, AFM revealed the binding of a bitter peptide (VAPFPEVF) to its receptor (TAS2R16) without triggering downstream signaling. It also sheds light on oral texture perception, which remains underexplored at the biomolecular level [1]. By combining AFM with biochemical assays, molecular simulations, and human sensory evaluations, this research bridges objective measurements and subjective flavor experiences. These findings offer new approaches to designing healthier, sensory-appealing foods, addressing critical health and nutrition challenges. [1] Koehler, M, et al. Nature Food (2024): 1-7.

BP 7.5 Mon 16:30 H44

Label-Free Photothermal Infrared Correlation Spectroscopy — •Arthur Markus Anton and Frank Cichos — Leipzig University, Peter Debye Institute for Soft Matter Physics, Linnéstr. 5, 04103 Leipzig

Correlation spectroscopy is an indispensable method in modern life science. It allows for retrieving analyte properties in solution like it's concentration or diffusion coefficient, and thus enables to calculate the hydrodynamic radius of proteins or the viscosity of membranes, for instance. Common techniques are based on fluorescence or scattering, such as fluorescence correlation spectroscopy or dynamic light scattering respectively, and therefore need fluorescent labeling of analytes or lack of molecular specificity.

In this contribution we present a novel spectroscopic correlation technique on the basis of pumping with IR light but probing by means of visible light. The absorption of IR light is highly specific and allows us for *label-free* addressing of specific vibrational modes within the analyte molecules via the particular pump wavelength. Upon absorption, energy is dissipated and transferred into heat which alters the refractive index of the medium surrounding the absorbing species. This *transient* refractive index change is then probed by means of visible light providing a similar probe focal volume as conventional correlation spectroscopy techniques. Consequently, on the basis of IR pumping and visible probing we calculate the analyte's concentration and diffusion coefficient.

BP 7.6 Mon 16:45 H44

Single-protein optical holography — •Jan Christoph Thiele[1,2], Emanuel Pfitzner[1,2], and Philipp Kukura[1,2] — [1]Kavli Institute for Nanoscience Discovery, University of Oxford, UK — [2]Department of Chemistry, University of Oxford, UK

Light scattering by nanoscale objects is a fundamental physical property defined by their scattering cross-section and thus polarizability. Over the past decade, a number of studies have demonstrated single-molecule sensitivity by imaging the interference between scattering from the object of interest and a reference field. This approach has enabled mass measurement of single biomolecules in solution owing to the linear scaling of image contrast with molecular polarizability. Nevertheless, all implementations so far are based on a common-path interferometer and cannot separate and independently tune the reference and scattered light fields, thereby prohibiting access to the rich toolbox available to holographic imaging. Here we demonstrate comparable sensitivity using a non-common-path geometry based on a dark-

field scattering microscope, similar to a Mach-Zehnder interferometer. We separate the scattering and reference light into four parallel, inherently phase-stable detection channels, delivering a five orders of magnitude boost in sensitivity in terms of scattering cross-section over state-of-the-art holographic methods. We demonstrate the detection, resolution and mass measurement of single proteins with mass below 100 kDa. Separate amplitude and phase measurements also yield direct information on sample identity and experimental determination of the polarizability of single biomolecules.

BP 8: Biomaterials, Biopolymers and Bioinspired Functional Materials I (joint session BP/CPP)

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

BP 8.1 Mon 15:00 H46

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

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

BP 8.2 Mon 15:15 H46

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

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

BP 8.3 Mon 15:30 H46

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

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

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

BP 8.4 Mon 15:45 H46

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

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

BP 8.5 Mon 16:00 H46

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

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

Invited Talk BP 8.6 Mon 16:15 H46

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

In vivo, cells and multicellular assemblies often experience strong confinement by their surrounding tissue environment, particularly in cancer. Thus, replicating these confined environments in situ is essential for investigating their impact on cellular systems. Using two-photon lithography, we printed structures directly within and around multicellular assemblies. For example, we fabricated dome-shaped confinements with micrometer-scale openings to encapsulate cancer spheroids. This enabled us to study how confinement influences cancer cell migration and spheroid behavior. Our findings revealed that confine-

ment slows cell migration and alters actin dynamics. In addition, in situ printed structures can also directly interfere with migrating cellular assemblies. Additionally, elastic structures can be created to mechanically stimulate cells, offering further control over cellular behavior. Therefore, two-photon lithography proves to be a powerful tool for manipulating the growth, migration, and morphology of live cells, making it particularly useful for exploring how changing physical microenvironment in situ affect cell responses.

BP 9: Biomaterials, Biopolymers and Bioinspired Functional Materials II (joint session CPP/BP)

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

BP 9.1 Mon 17:00 H46

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

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

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

BP 9.2 Mon 17:15 H46

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

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

BP 9.3 Mon 17:30 H46

Model particles to study interaction of microplastic particles — •Kai Gossen, Andreas Fery, and Günter Auernhammer — IPF Dresden, Dresden, Germany

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

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

BP 9.4 Mon 17:45 H46

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

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

BP 10: Focus Session: Nonlinear Dynamics in Biological Systems I (joint session DY/BP)

Nonlinear dynamics play a central role for biological systems to achieve remarkable complexity and adaptability. They underlie processes where small changes cascade into large effects, critical thresholds drive transitions, and feedback mechanisms maintain intricate balances. Biological systems are often far from equilibrium, exhibiting behaviors shaped by competing forces, stochastic fluctuations and emergent behavior. From the amplification of sensory signals near bifurcation points to the development of turbulence, concepts from nonlinear dynamics provide a unifying framework for studying patterns, stability, and collective behavior in living systems. This focus session explores the richness of nonlinear dynamics across biological scales, from molecular circuits to population-level phenomena, spanning vastly different fields from cardiac dynamics, embryogenesis and cell motility to active fluids, condensates and origin of life. Through theoretical models, experimental insights, and computational approaches, the talks illustrate how nonlinear-dynamics principles unravel the mechanisms driving function and complexity in biology, offering new perspectives across disciplines.

Organized by Philip Bittihn (Göttingen), Stefan Klumpp (Göttingen), and Carsten Beta (Potsdam)

Time: Tuesday 9:30–12:30 Location: H43

Invited Talk BP 10.1 Tue 9:30 H43

Robust signal amplification and information integration via self-tuned proximity to bifurcation points — •Isabella Graf — Developmental Biology Unit & Theory Transversal Theme, EMBL Heidelberg, Germany

Many living systems demonstrate exquisite sensitivity to small input signals. A tempting hypothesis is that these systems operate close to bifurcation or critical points, where the system's response exhibits a diverging susceptibility to the control parameter and small signals are amplified into a large collective response. A common concern, however, is that proximity to such points requires fine-tuning of parameters, which seems impossible for noisy biological systems. Based on several distinct sensory systems, we have investigated a feedback motif that robustly maintains these systems close to their respective bifurcation point. The key ingredient is that the collective response feeds back onto the control parameter. To illustrate this idea, I will mention several examples ranging from snake thermosensing to mammalian hearing and discuss the functional benefits associated with being near-critical.

BP 10.2 Tue 10:00 H43

Exceptional Points and Stability in Nonlinear Models of Population Dynamics having PT symmetry — •Alexander Felski — Max Planck Institute for the Science of Light, Erlangen, Germany

Nonlinearity and non-Hermiticity, for example due to environmental gain-loss processes, are a common occurrence throughout numerous areas of science. For the latter, parity-time-reflection (PT) symmetry has played an eminent role in understanding exceptional-point structures and phase transitions in these systems. Yet their interplay has remained by-and-large unexplored. We analyze models governed by the replicator equation of evolutionary game theory and related Lotka-Volterra systems of population dynamics. These foundational nonlinear models offer a broad platform for non-Hermitian theory beyond physics. In this context we study the emergence of exceptional points in two cases: (a) when the governing symmetry properties are tied to global properties of the models, and, in contrast, (b) when these symmetries emerge locally around stationary states–in which case the connection between the linear non-Hermitian model and an underlying nonlinear system becomes tenuous. We outline further that when the relevant symmetries are related to global properties, the location of exceptional points in the linearization around coexistence equilibria coincides with abrupt global changes in the stability of the nonlinear dynamics. Exceptional points may thus offer a new local characteristic for the understanding of these systems.

BP 10.3 Tue 10:15 H43

Pattern selection and the route to turbulence in polar active fluids — Henning Reinken[1], Sebastian Heidenreich[2], •Markus Bär[2,3], and Sabine Klapp[3] — [1]OVGU Magdeburg, Germany — [2]Physikalisch-Technische Bundesanstalt, Germany — [3]TU Berlin, Germany

Active fluids, such as suspensions of microswimmers, are well known to self-organize into complex spatio-temporal flow patterns. An intriguing example is mesoscale turbulence, a state of dynamic vortex structures exhibiting a characteristic length scale. Here, we employ a minimal model for the effective microswimmer velocity field to explore how the turbulent state develops from regular, stationary vortex patterns when activity is increased. First, we demonstrate analytically that the system develops a stationary square vortex lattice in the absence of nonlinear advection. Subsequently, we perform an extended stability analysis and uncover a linear instability, above which the square vortex lattice becomes unstable. In numerical simulations, we confirm that this instability is predictive for the unset of turbulence. In addition, an extended region of hysteresis where turbulence and a stable vortex lattice coexist, is found Reference: H. Reinken, S. Heidenreich, M. Bär, S. Klapp, New J. Phys. 26 063026 (2024).

BP 10.4 Tue 10:30 H43

Likelihood-based inference for heterogeneous motile particle ensembles — •Jan Albrecht[1], Cristina M. Torres[1], Carsten Beta[1], Manfred Opper[2,3,4], and Robert Grossmann[1] — [1]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [2]Faculty of Electrical Engineering and Computer Science, Technische Universität Berlin, 10587 Berlin, Germany — [3]Centre for Systems Modelling and Quantitative Biomedicine, University of Birmingham, B15 2TT, United Kingdom — [4]Institute of Mathematics, University of Potsdam, 14476 Potsdam, Germany

The inherent complexity of biological agents often leads to motility behavior that appears to have random components. Robust stochastic inference methods are therefore required to understand and predict the motion patterns from time discrete trajectory data provided by experiments. In many cases second-order Langevin models are needed to adequately capture the motility. Additionally, population heterogeneity needs to be taken into account when analyzing data from multiple individual organisms. We present a maximum likelihood approach to infer stochastic models and, simultaneously, estimate the heterogeneity in a population of motile active particles from discretely sampled trajectories. To this end we propose a new method to approximate the likelihood for nonlinear second order Langevin models. We demonstrate that our approach outperforms alternative methods for heterogeneity estimation, especially for short trajectories, while also providing a measure of uncertainty for the estimates. We use the approach to investigate population heterogeneity in systems of ameboid cells.

BP 10.5 Tue 10:45 H43

Surviving the first "winter": Protocells with polymerization reactions protects against environmental fluctuations — •Xi Chen, Jens-Uwe Sommer, and Tyler Harmon — Leibniz Institute of Polymer Research, Dresden, Germany

The origin of life has been a long standing question with various hypotheses describing the emergence of the first protocells. Phase separated condensates are promising candidates for protocells because they are compartments that enrich specific polymers and host nonequilibrium reactions that leads to growth and division. However, the ability of protocells to survive in an environment that has large fluctuations, such as temperature and composition, is poorly understood. We show with a mean-field model that condensates formed by polymers which undergo nonequilibrium polymerization/depolymerization reactions exhibit significant robustness to large environmental fluctuations.

This robustness occurs when the nonequilibrium polymerization reactions are faster inside condensate phases than outside. The first

condensate does not form until environmental factors lead to strong enough reactions that polymers long enough to phase separate form. The effects of nonequilibrium polymerization is then fully realized because a condensate exists. From here, the condensate does not dissolve until the nonequilibrium reactions are diminished to significantly below when the condensate formed. Altogether, this forms a hysteretic loop with respect to the environmental factors that drive nonequilibrium reactions. We show this hysteretic loop prevents protocells from dying from environmental fluctuations.

BP 10.6 Tue 11:00 H43

How inter-particle interaction affects two species transport in nano-channels — •Wolfgang Bauer — Dept. of Internal Medicine I, UKW, Würzburg, Germany

Channel transport mechanisms of multiple species is essential for cell physiology and nanotechnology. Here, we present a model maintaining spatial correlations of two species, moving away from mean field approaches. The spatial occupations of the channel give the state space, where local flux and entropy production determine channel transport and its thermodynamic efficiency. Optimal transport coupling between species occurs in an attractive empty channel and strong repulsive forces between particles of the same species. This confines state space to a circular topology with concentration gradients of the two species acting as thermodynamic driving forces in series. For opposing gradients, the species with the stronger gradient produces positive entropy, while the other negative entropy. Attenuating the repulsive force within one species and maintaining that of the other adds a bypass path on the circular topology in state space. This enables a leak flow of the less repulsive species parallel to its gradient, generating local positive entropy on the bypass. For a certain range of opposing gradients, both species can produce positive overall entropy simultaneously. However, the rectifying potential of the concentration gradient of the species with bypass option is diminished, i.e. it cannot rectify flow of the other species above a threshold of the latter's opposing gradient. Vice versa the flow of the species with bypass option may always be rectified parallel to the concentration gradient of the other.

15 min. break

Invited Talk BP 10.7 Tue 11:30 H43

Beyond the connectionist view: (De-)synchronizing neural networks via cell-intrinsic dynamics — •Susanne Schreiber — Humboldt-Universität zu Berlin, Institute for Theoretical Biology, Berlin, Germany

Neural computation is thought to arise from the connectivity among neurons. Accordingly, we are often more than happy to ignore seemingly unimportant and potentially overwhelming biological detail, for example, related to the properties of the neurons themselves. In this talk, however, I will highlight how cell-intrinsic dynamics, namely the biophysics of action-potential generation, can have a decisive impact on network behaviour. Recent work of my lab shows that, among regularly firing neurons, the somewhat unattended homoclinic type (characterized by a spike onset via a saddle homoclinic orbit bifurcation) particularly stands out: First, spikes of this type foster specific network states - synchronisation in inhibitory and splayed-out/frustrated states in excitatory networks. Second, homoclinic spikes can be easily induced in by changes in a variety of physiological parameters (like temperature, extracellular potassium, or dendritic morphology). As a consequence, small changes in these parameters can suffice to induce drastic switches in network states. I will discuss functional consequences of homoclinic spikes for the design of pattern-generating motor circuits in Drosophila as well as for mammalian pathologies like febrile seizures. Our work predicts an interesting role for homoclinic action potentials as an integral part of brain dynamics in both health and disease.

BP 10.8 Tue 12:00 H43

Transient spatiotemporal chaos in cardiac excitable media — •Melvin Dix[1,2], Thomas Lilienkamp[1,3], Stefan Luther[1,4,5], and Ulrich Parlitz[1,2,5] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, Georg-August-Universität Göttingen, Göttingen, Germany — [3]Faculty for Applied Mathematics, Physics, and General Science, Computational Physics for Life Science, Nuremberg Institute of Technology Georg Simon Ohm, Nürnberg, Germany — [4]Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Göttingen, Germany — [5]German Center for Cardiovascular Research (DZHK), Partner Site Göttingen, Göttingen, Germany

Life-threatening cardiac arrythmia such as ventricular fibrillation have been linked to spatiotemporal chaotic dynamics governed by scroll or spiral waves. It has been observed in vivo and in vitro that these dynamics can be transient, e.g. abruptly stop. Using simulations with different numerical models we investigate the effects of factors such as heterogeneities, motivated by the complexity of the heart. We show that these perturbations can (significantly) prolong the duration of chaotic transients and may also lead to persistent chaos or stable periodic wave patterns [1].

[1] Melvin Dix et al. Physical Review E 110(4), 044207 (2024).

BP 10.9 Tue 12:15 H43

Nonlinear dynamics of heart and brain — •Irene Pellini[1,2], Simon Bauer[1], Johannes Zierenberg[1,3], Philip Bittihn[1,3], and Viola Priesemann[1,3] — [1]Max Planck Institute for Dynamics and Self Organisation, Göttingen, Germany — [2]Max Planck School Matter to Life, Heidelberg, Germany — [3]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

The core function of the heart and brain arises from the coordinated interaction of their cells. Both organs rely on excitable units – cardiomyocytes and neurons – that propagate electrical signals when a specific threshold is exceeded. Despite this similarity, the two organs exhibit opposed collective behavior due to marked differences in intercellular dynamics and network topology. In the heart, localized electrical connectivity through reciprocal gap junctions generates local synchronization and traveling waves, ensuring efficient pumping function with low entropy. In the brain, long-range connectivity via delayed, non-reciprocal chemical synapses promotes asynchronous dynamics with high entropy, supporting information processing.

Using coupled FitzHugh-Nagumo oscillators, we showcase that characteristic non-linear dynamics for the heart and brain can be related to the network structure, which places both systems on opposite sides of a synchronization phase transition. Crossing this phase transition would lead to pathological conditions, e.g., heart arrhythmia or brain seizures, quantifiable via entropy measures. Our joint view on heart and brain dynamics may foster new perspectives on the function and pathology of both organs.

BP 11: Cytoskeleton

Time: Tuesday 9:30–11:30 Location: H44

Invited Talk BP 11.1 Tue 9:30 H44

Network connectivity determines the mechanisms responsible for cytoskeletal elasticity — •Martin Lenz — Université Paris-Saclay, CNRS, LPTMS, 91405, Orsay, France — PMMH, CNRS, ESPCI Paris, PSL University, Sorbonne Université, Université Paris-Cité, F-75005, Paris, France

Much of the cell's mechanics is dictated by the properties of its cytoskeleton, a dynamic collection of semiflexible filaments. Here we review both old and new results on the emergence of its large-scale elasticity from the filaments' individual mechanical properties. We emphasize the role of the network's connectivity in determining the underlying physical mechanism. At high connectivity or under high stress, the tensile strength of the filaments dominate. Moderately coordinated networks, on the other hand, are governed by the filaments' bending elasticity. Finally, we discuss the very low coordination of branched actin networks, and argue that it implies that interfilament contacts play a major role in its response. This makes the mechanics of these networks analogous to that of a ball of unspun sheep's wool under compression.

BP 11.2 Tue 10:00 H44

Buckling action of molecular motors damages microtubules beyond self-repair — •Shweta Nandakumar[1], Jonas Bosche[1], Morgan Gazzola[2], Mirko Wieczorek[1], Mona Grünewald[1], Manuel Thery[2], Reza Shaebani M[1], Ludger Santen[1], Stefan Diez[3], and Laura Schaedel[1] — [1]Center for Biophysics, Saarland University, Germany — [2]IPGG, Paris, France — [3]B-CUBE,TUD Dresden. Germany

Microtubules (MTs) are rigid, hollow biopolymers that constitute a key component of the cytoskeleton, essential for cellular processes such as mitosis, intracellular transport, and migration. Despite their large bending rigidity, MTs often adopt highly curved conformations, indicating that they are exposed to significant mechanical forces in cells. These forces typically arise from molecular motor proteins like kinesin.

In this study, we investigated microtubule damage and subsequent self-repair as a result of both bending as well as dynamic buckling using kinesin motor proteins in vitro. We reveal that motor-induced buckling imposes massive damage on MTs, occasionally leading to the renewal of majority of the MT lattice visualised by the incorporation of new tubulin subunits into the damaged regions. We find that at high motor densities, MT damage exceeds self-repair and leads to frequent MT breakage.

Our results highlight the impact of mechanical forces, which significantly speed up MT damage and self-repair, on MT integrity. Our findings provide a framework for understanding how cells maintain MT function under repeated mechanical stress.

BP 11.3 Tue 10:15 H44

Active self-organization of focal adhesions driving cell shape changes — •waleed ahmad mirza, matt govendir, alejandro torres-sánchez, and maria bernabeu — European Molecular Biology Laboratory, Barcelona

Focal adhesions (FAs) are dynamic protein complexes that mediate the interplay between the actin cytoskeleton and the extracellular matrix (ECM), enabling cells to sense and respond to mechanical and biochemical cues. These complexes drive essential processes such as cytoskeletal reorganization, cell shape modulation, and migration. To investigate these processes, we developed an active gel mathematical model that couples the dynamics of FAs, actin cytoskeleton, and cellular shape changes, capturing the three-way interplay between these components. Numerical solutions of the model successfully recapitulated experimental observations, demonstrating its ability to predict how cells adapt to mechanical and topographical cues. Specifically, the model reproduced key phenomena such as the influence of substrate stiffness on FA dynamics, with stiffer substrates promoting larger, more stable FAs, aligned stress fibers, and enhanced cell motility. It also captured how anisotropic ECM features, such as aligned collagen fibers or patterned topography, direct cytoskeletal organization and cell alignment. Additionally, the model demonstrated how curvature and shear flow provide critical mechanical cues that shape cellular morphology and behavior. This work provides a novel framework for understanding the mechanistic feedback loops underlying cell-ECM interactions and highlights the central role of FAs in regulating cellular behavior.

BP 11.4 Tue 10:30 H44

Interactions between single actin and vimentin filaments — •Pallavi Kumari and Sarah Köster — Institute for X-Ray Physics, University of Göttingen, Germany

The cytoskeleton plays a crucial role in maintaining cellular structure, mechanics, and function. Recent advances suggest that the diverse tasks of the eukaryotic cytoskeleton depend on the interactions between its filamentous components - microtubules, actin filaments, and intermediate filaments. Despite a growing number of studies to better understand these interactions, it remains unclear whether actin and intermediate filaments interact directly without an auxiliary protein. Previous in vitro studies on reconstituted mixed filament networks have reported contradictory results. To clearly resolve this contradiction, it is essential to further simplify the system down to the single filament level. Here, we present a study on the direct interactions between actin filaments and vimentin intermediate filaments at the single filament level, examining the effects of different ions at varying concentrations on the interaction force. We employ quadruple optical tweezers combined with confocal microscopy and microfluidics to precisely control the conditions for the interaction of the two reconstituted protein filaments, visualize the interactions, and measure the forces involved. Our research provides direct indications of interactions between actin and vimentin filaments. Our findings will provide important insight that will help to unravel the interplay of cytoskeletal filaments at the network level.

BP 11.5 Tue 10:45 H44

Active Gel Theory for Cell Migration With Two Myosin Species — •Nils Winkler, Oliver M Drozdowski, Falko Ziebert, and Ulrich S Schwarz — Institut für theoretische Physik und Bioquant, 69120 Heidelberg

Motility of animal cells is essential for a wide range of biological phenomena, from the development of embryos to the spread of cancer. It is mainly driven by flow of the actin cytoskeleton, which in turn is generated by both actin polymerization and actomyosin contractility. Non-muscle myosin II is present in three different isoforms, but it is unclear what their respective roles are. Starting from phenomenological binding kinetics that include the competition of the myosin motors for binding sites through excluded volume interactions, we derive an active gel model for cell migration that includes a fast and a slow variant, corresponding to the non-muscle myosin II isoforms A and B, respectively. We find non-linear diffusion laws and predict species gradients that agree with experimental observations. Through numerical continuation and simulations, we identify a pull-and-push mechanism that can produce different system states, including steady migration as well as cell oscillations in length and velocity.

BP 11.6 Tue 11:00 H44

Keratin networks in epithelial cells under strain — •Ruben Haag, Ruth Meyer, and Sarah Köster — Institute for X-Ray Physics, University of Göttingen, Germany

The cytoskeleton is mainly made up of microtubules, actin and intermediate filaments (IFs). The composition of the IF-network is cell-type specific and influences the viscoelastic properties of cells. In epithelial cells, the keratin IF network connects to desmomes in the cell membrane, while in the cell center keratin IFs can bind to the nuclear lamina via plectin proteins. The keratin IF network thus forms a mechanical link from the nucleus to the cell membrane. In in-vitro experiments, it was previously observed that IFs, unlike actin filaments, resist being stretched to high strains. We now ask whether this force-extension behavior of IFs is also relevant in whole cells and, more specifically, if mechanical signals from outside the cell are transmitted to the nucleus via the keratin IF network. To answer this question, we stretch cells both uniaxially to linear strains of 80 % and equibiaxially to area strains of 87 %. During stretching, we image the nuclei, deconvolve the images to recover their 3D shape, segment the nuclei and track each nucleus during stretching. This procedure allows us to investigate their deformation at increasing strain. We compare wild type epithelial cells to keratin knockout cells to study the influence of the keratin IF network on the nuclei. We find that the deformation orthogonal to the

stretching direction of the nuclei matches the deformation of the cell better in the keratin wild type cells. Our results suggest, that the keratin network helps to adapt the nucleus to mechanical perturbation.

BP 11.7 Tue 11:15 H44

Investigating the interaction between two single heart cells through TNTs using ROCS and Fluorescence microscopy — •Arash Felekary and Alexander Rohrbach — Lab for Bio and Nano Photonics, IMTEK, Freiburg, Germany

Cell-cell communication is vital for biological processes, particularly in the heart. Tunneling nanotubes (TNTs), dynamic and thin protrusions, facilitate cellular interactions by transferring organelles, including mitochondria. To investigate TNT composition and their roles in cardiac fibroblast (FB) communication, we employed Rotating Coherent Scattering (ROCS) microscopy, a label-free super-resolution technique, in addition to Fluorescence microscopy. ROCS enables up to 100 Hz recordings of lamellipodia dynamics along TNTs, and 3D imaging across different z-planes up to 6μm in depth, which is critical for visualizing TNTs. We observed a linear correlation between TNT density and lamellipodia motion velocity. Lamellipodia, driven by actin polymerization and branching via Arp2/3 activation, play a key role in FB migration and interaction. Collagen staining demonstrated that TNTs and lamellipodia interact with collagen fibers, a major component of the extracellular matrix (ECM). This interaction not only influences ECM remodeling, but also activates actin branching signals that enhance FB migration and protrusion dynamics. In this presentation, we investigate the coordinated roles of TNTs, lamellipodia, and collagen in regulating FB interaction and migration, offering new insights into heart tissue repair.

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

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

Invited Talk BP 12.1 Tue 9:30 H46

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

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

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

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

BP 12.2 Tue 10:00 H46

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

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

BP 12.3 Tue 10:15 H46

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

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

BP 12.4 Tue 10:30 H46

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

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

BP 12.5 Tue 10:45 H46

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

Foams consist of foam lamellas, which separate single air bubbles from

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

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

BP 12.6 Tue 11:00 H46

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

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

BP 13: Active Matter III (joint session DY/BP/CPP)

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

BP 13.1 Tue 9:30 H47

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

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

BP 13.2 Tue 9:45 H47

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

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

BP 13.3 Tue 10:00 H47

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

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

[1] T. Vicsek, Phys. Rev. Lett. 75, 1226 (1995).
[2] O. Chepizhko, E. G. Altmann, and F. Peruani, Phys. Rev. Lett. 110, 238101 (2013).

BP 13.4 Tue 10:15 H47

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

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

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

taxis, enabling the swimmers to avoid dead ends and autonomously find paths through complex mazes.

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

BP 13.5 Tue 10:30 H47

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

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

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

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

Invited Talk BP 13.6 Tue 10:45 H47

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

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

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

15 min. break

BP 13.7 Tue 11:30 H47

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

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

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

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

BP 13.8 Tue 11:45 H47

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

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

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

BP 13.9 Tue 12:00 H47

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

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

BP 13.10 Tue 12:15 H47

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

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

Invited Talk BP 13.11 Tue 12:30 H47

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

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

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

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

BP 14: Poster Session I

Bacterial biophysics, computational biophysics, membranes and vesicles, synthetic life-like systems and origin of life, systems and networks biophysics

Time: Tuesday 10:00–12:30 Location: P3

BP 14.1 Tue 10:00 P3

The Role of Localized Metabolic Activity in Streptomyces Hyphae: An Agent-Based Approach — •Ricardo Santander[1], Denis Iliasov[2], Thorsten Mascher[2], and Vasily Zaburdaev[1] — [1]Max-Planck Zentrum für Physik und Medizin, Kussmaulallee 2, Erlangen — [2]Institut für Mikrobiologie, Zellescher Weg 20b, Dresden

The filamentous bacterium Streptomyces undergoes complex multicellular development characterized by hyphal growth and branching. Recent discoveries of LpdA-containing fluorescent foci within the hyphae suggest localized sites of elevated metabolic activity and ATP production. To investigate their influence on hyphal morphogenesis, we developed an agent-based model simulating key cellular components and their interactions.

Simulations reveal that localized ATP production and high consumption rates near the tips create spatial heterogeneity in metabolic activity. By adjusting model parameters, the model replicates typical growth patterns and hyperbranching phenotypes observed experimentally.

Our findings suggest that the spatial distribution of metabolic foci and localized ATP production influence Streptomyces morphology and multicellular organization.

BP 14.2 Tue 10:00 P3

Optically driven thermofluidic assembly of bacteria — •Desmond Joseph Quinn[1], Selina Hanisch[2], Rohan Karande[3], and Frank Cichos[1] — [1]Peter Debye Institute for Soft Matter Physics, Faculty of Physics and Earth Sciences, Leipzig University, Leipzig, Germany — [2]Helmholtz Center for Environmental Research (UFZ), Leipzig, Germany — [3]Biophysical Chemistry, Leipzig University, Leipzig, Germany

Bacteria in their planktonic state are known to assemble into biofilms in the vicinity of a solid surface. The complex cascade that results in the adhesion of the bacteria to the surface is usually triggered by the diffusion of bacteria to its vicinity. We propose a method that makes use of temperature induced flow fields and depletion interactions for the localized assembly and manipulation of bacteria. In addition to the physical interactions that contribute to the assembly process, the motility of the bacteria affects the assembly and can be altered by the induced temperature and altered distribution of molecules. We try to disentangle these effects by studying passive and active bacteria independently. We look at how motility parameters change in response to the fields induced by the laser, and how this in turn affects assembly. Such controlled assembly of bacteria could be useful for technological applications in bioreactors. In addition, our method provides a way of experimentally probing the effect of localized temperature, osmotic pressure, and flow fields on the motility of bacteria.

BP 14.3 Tue 10:00 P3

Growth and characterization of MoS2 nanowalls on Ti-based bone implants — •Rania Ennaciri, Axel Printschler, Christof Neumann, and Andrey Turchanin — Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany

Antibiotic resistance presents an important issue in the medicine field particularly in the context of bone replacement surgeries, where infections from antibiotic-resistant bacteria can lead to severe health complications and even fatalities. While titanium (Ti) is the conventional choice for bone implants, there is a clear need for further improvements of this material to enhance its antimicrobial resistance. In this regard, hybrids based two-dimensional (2D) materials, such as molybdenum disulfide (MoS2), present a great promise due to their intrinsic antimicrobial activity and biocompatibility. These properties are generally manifested through biochemical reactions, by the generation of reactive oxygen species (ROS) that can lead to the damage of bacteria DNA, proteins and lipids. Also, mechanical actions, where the sharp edges of the nanowalls can cut the bacteria wall can lead to its death. To investigate these mechanisms, we use metal-organic chemical vapor deposition (MOCVD) technique to grow different morphologies and sizes of MoS2 nanowalls on Ti implants. We use scanning electron microscope (SEM), Raman spectroscopy and X-ray electron microscopy (XPS) to characterize the structural and chemical properties and to correlate them prospectively with the antimicrobial properties as well as with the growth bone cells.

BP 14.4 Tue 10:00 P3

Infrared Hyperspectral Mapping of Biofilms Growing in Confinement — •Felix Hermann Patzschke[1], Valentina Schmitz[2], Rohan Karande[2,3], and Frank Cichos[1] — [1]Leipzig University, Peter Debye Institute for Soft Matter Physics, Linnéstr. 5, 04103 Leipzig — [2]Leipzig University, Institute for Biochemistry, Johannisallee 21-23, 04103 Leipzig — [3]Helmholtz Centre for Environmental Research, Permoserstraße 15, 04318 Leipzig

Biofilms are microbial communities characterized by complex spatial organization and dynamic chemical composition. The formation and growth of biofilms in confined environments are of significant interest in fields such as medicine and bio-engineering. We seek to establish a clearer understanding of the interplay between physical confinement and microbial behavior by investigating whether specific quantifiable aspects of a cavity's geometry can influence the likelihood of biofilm initiation and the rate of its growth.

We utilize Photothermal Infrared (PTIR) hyperspectral microscopy to acquire infrared spectral data at sub-cellular spatial resolutions. Through spectral decomposition, we aim to map the chemical composition of biofilms and distribution of nutrients in space and time. Our results provide a detailed view of biofilm structure, metabolic activity, and growth dynamics in confined settings. This work underscores the potential of PTIR microscopy as an impactful tool for advancing the understanding of biological systems in scientifically and technologically significant domains.

BP 14.5 Tue 10:00 P3

Self-Organized Colonization Resistance without Physical Barriers — •Christian Westendorf[1], Valentin Slepukhin[1], Birgit Koch[1], Victor Peris[1], and Oskar Hallatschek[1,2] — [1]Peter Debye Institute for Soft Matter Physics, Leipzig University. — [2]Department of physics, University of California, Berkeley.

Small micrometer-scale cavities, such as gut crypts, soil pores, and plant apoplasts, represent key bacterial habitats, in which different strains compete for resources and space. Recent studies have shown that the physical structures of these microhabitats can influence the stability and resilience of bacterial colonizers by protecting local populations from invasion. Building on this, we experimentally and computationally investigate the dynamics of mixed bacterial populations within interconnected microfluidic cavities, examining the influence of geometric features and surface interactions on microbial organization and diversity. Our findings reveal that surface roughness and friction can drive self-organization into effectively isolated subpopulations, safeguarding slower-growing strains from competitive exclusion. By comparing velocity fields of growing populations with stochastic and analytical simulations, we demonstrate how local geometry and emergent microhabitats balance selective pressures, maintaining mi-

crobial diversity under competitive and evolutionary stress. Our work suggests that colonization-resistant microhabitats can form dynamically, even in the absence of physical barriers.

BP 14.6 Tue 10:00 P3

Comparing graphene and 2D MoS_2 nanopores for protein translocation and detection — •Peijia Wei, Mayukh Kansari, and Maria Fyta — Computational Biotechnology, RWTH Aachen University, Worringerweg 3, 52074 Aachen, Germany

Nanopores, nanometer-scale openings in materials, have shown their strong potential in realizing ultra-fast, cost-effective, and real-time next-generation sequencing technology. These nanopores can electrophoretically drive charged biomolecules and detect these. Using computer simulations, we compare two-dimensional nanopores, namely graphene and MoS_2, to evaluate their effectiveness in protein detection. We modulate protein translocation and dynamics by adjusting the type and concentration of the surrounding solvent, using a typical monovalent salt solution and a molecular solution. Utilizing atomistic simulations, we assess the efficiency of both nanopores in threading proteins, based on measurable ionic current signals. Our results show that graphene nanopores strongly interact with proteins, hindering translocation under physiological conditions. This issue is addressed by introducing a denaturant, which creates a hydrophilic-cationic layer on the pore surface, facilitating the linearized threading of proteins. In contrast, MoS_2 nanopores facilitate protein passage even in physiological solutions, offering an alternative approach to controlling translocation speed. We analyze the two nanopore materials based on molecular interactions among the material, protein, and solvent, emphasizing their impact on protein dynamics and ionic signal enhancement for efficient 2D nanopore protein detection.

BP 14.7 Tue 10:00 P3

Exploring coarse graining RNA force fields via Machine Learning — •Anton Dorn[1] and Alexander Schug[1,2] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]KIT Scientific Computing Center, Karlsruhe, Germany

In Protein structure prediction there have been massive improvements recently with the help of machine learning. In RNA structure prediction however the situation is less ideal due too much sparser experimental data. Here we attempt to solve a modified version of the problem by determining a coarse-grained RNA force field for Molecular Dynamics simulations. The data sparsity can here be alleviated by atomistic RNA simulations using proven and established force fields. In a first step we show the viability of this approach with a limited scenario of only small RNA molecules. For this we adapt the invariant Graph Neural Network architecture, cgSchnett.

BP 14.8 Tue 10:00 P3

Parameterization of a dissipative particle dynamics thermostat (DPD) thermostat for coarse-grained molecular dynamics — •Karan Venkatesh, Viktor Klippenstein, and Nico F. A. van der Vegt — Technische Universität Darmstadt

Coarse-grained (CG) simulations represent a viable approach for modelling dynamics on long length and time scales inaccessible with atomistic simulations. In this work, we present a single-site coarse-graining method designed to match the dynamical and structural properties of a molecular liquid (cyclohexane).

We employ a DPD thermostat, in which the pairwise forces are decomposed into parallel and perpendicular components. An iterative optimization scheme is implemented to parameterize the parallel and perpendicular forces, aiming to match the diffusion coefficient and shear viscosity of the system, respectively. In our study, we find that matching the diffusion coefficient also leads to a match in the shear viscosity. However, this correspondence may not always hold, especially when dealing with structurally anisotropic molecules and soft potentials, as commonly encountered in soft matter systems. This approach can be further extended to simulate mixtures of CG molecular liquids, and study penetrant dynamics in CG polymer melts.

References: 1. V. Klippenstein; N F A van der Vegt; J. Chem. Theory Comput. 2023, 19(4), 1099-1110. 2. M. Tripathy; V Klippenstein; N F A van der Vegt; J. Chem. Phys. 2023, 159(9) 3. C. Junghans; M. Praprotnik; K. Kremer; Soft Matter 2008, 4(1), 156-161

BP 14.9 Tue 10:00 P3

Leveraging Experimental Vasculature Data for High Resolution Brain Tumor Simulations — •Eric Behle[1], Julian Herold[2], and Alexander Schug[1] — [1]NIC Research Group Computational Structural Biology, Jülich Supercomputing Centre, Jülich Research Center, Jülich, Germany — [2]Steinbuch Centre for Computing, KIT, Karlsruhe

Cancer remains a leading cause of mortality. Multidisciplinary studies probe its pathology to increase treatment options. Computational modeling of tumors on HPC resources offers insight into its progress and an avenue for advancing our understanding. However, initialization and parameterization of the underlying models require high-resolution data from real tissue structures. Here, we leveraged HPC resources and a massive dataset of a mouse brain's entire vascular network. We processed these image stacks into detailed 3D representations, identified brain regions of interest, and conducted a series of large-scale simulations to investigate how tumor growth is influenced by local vascular network characteristics. By simulating tumor growth with sub-cellular resolution, we can probe to which extent vessel density and network length influence growth. We determined that vessel density is the primary determinant of growth rate. Finally, our results allowed us to extrapolate tumor cell growth predictions for the entire mouse brain, highlighting the critical role of vascular topology in tumor progression. Such increasingly realistic simulations of cancer cells may enable researchers to bridge the gap between basic biology and clinical practice, supporting development of cancer therapies.

BP 14.10 Tue 10:00 P3

Boundary integral method for elastic solids in Stokes flow and applications in real-time deformability cytometry — •Thomas Mayr and Stephan Gekle — Universität Bayreuth, Deutschland

A Newtonian fluid at small Reynolds numbers can be described using the Stokes equation. A common choice to solve the Stokes equation numerically is the boundary integral method. Previously, this method was mainly used to describe rigid particles or capsules with an elastic membrane such as red blood cells. Here a technique is presented how to extend the boundary integral method to elastic solids discretized by the finite element method. This can be used as simple model to describe the stiffness of cells with a nucleus and a cytoskeleton, e.g. in some deformation experiments. In our case we will compare the simulations with an experimental technique called real-time deformability cytometry (RT-DC).

BP 14.11 Tue 10:00 P3

Mathematical Modeling of Intercellular Calcium Waves in Fibroblast Networks — •Kara Nachtnebel — Isarstr, 6, 93057 Regensburg

Inflammatory responses are essential for defending against pathogens but can result in tissue damage when not properly regulated. Resident tissue macrophages (RTMs) play a crucial role in maintaining immune homeostasis by modulating inflammatory cascades. Disruptions in these regulatory mechanisms can lead to heightened immune responses and may contribute to the development of autoimmune diseases. This study explores the role of fibroblast networks and their calcium signaling dynamics in maintaining tissue homeostasis. We aim to understand the mechanisms underlying these dynamics and predict calcium signal propagation in both healthy and pathological tissues. A mathematical model is developed to describe intracellular calcium ion diffusion and Inositol-1,4,5-triphosphate (IP3) signaling in fibroblast cells interconnected by gap junctions (GJs). This model incorporates intracellular calcium stores and IP3-sensitive receptor (IPR) dynamics, which significantly influence calcium release into the cytoplasm. IP3 generation is modeled as a function of phospholipase-C (PLC) activation, triggered either by external stimuli or by calcium, leading to calcium-induced calcium release (CICR). Our approach provides insights into how calcium signaling networks contribute to tissue homeostasis and how their dysfunction occurs in pathological conditions.

BP 14.12 Tue 10:00 P3

coarse-grained simulations of Lge1(1-80) peptide. — •Agaya Johnson[1], Anton Polyansky[2], Pedro Sanchez[1], Bojan Zagrovic[2], and Sofia Kantorovich[1] — [1]Computational and soft matter physics, University of Vienna, Kolingasse 14-16, 1090, Vienna, Austria. — [2]Department. of structural and computational biology, Campus- Vienna-biocenter 5, 1030 Vienna, Austria.

Biomolecular condensates in cells such as p-bodies, nucleoli and stress granules play an important role in regulating biological processes like transcription and ribosome biogenesis. Studying of such biomolecular condensates will give insight into the molecular basis of disease, like neurodegenerative diseases, cancer and diabetes. The main purpose of

this study is to understand the main phenomenon, which leads to the formation of these biomolecular condensates such that we get a conclusion, whether is it phase separation, self-assemble or an aggregation. We use Lge1(1-80) peptide as a model for study because Lge1(1-80) is mostly disordered prone to form many cation - pi and pi - pi interaction (R, G and Y rich sequence) and because of its alternating net charge which are the prerequisites for the phase separation. Due to the limitations of high-resolution experimental techniques, we are using molecular dynamics simulation with coarse-grained approaches with the help of software package ESPResSo. Our goal is to develop a coarse-grained model for proteins that exhibit structural transitions and to understand fundamental mechanisms under those transitions.

BP 14.13 Tue 10:00 P3

Optimizing a Biomimetic Cross-Flow Microplastics Filter Inspired by Manta Rays — •Ioannis Gkekas[1] and Tim Robertino Baumann[2] — [1]Universität Bielefeld — [2]Universität Bielefeld

Microplastic pollution poses a significant threat to aquatic ecosystems, necessitating innovative filtration solutions. This study continues previous research on a biomimetic cross-flow filter inspired by manta ray feeding mechanisms. The objective is to optimize the filter's geometry and material properties to enhance efficiency and durability. Using COMSOL simulations, various geometrical configurations are being tested to identify an optimal design for maximizing filtration efficiency and clean water output. To address material durability, we reenforced PDMS (polydimethylsiloxane) with glass fibers to mitigate bursting under operational stress. Initial results indicate that the composite material significantly enhances durability compared to the original PDMS design. Once the simulations are complete, the optimal design will be fabricated for in-lab performance evaluation. This research advances the development of sustainable, high-efficiency microplastic filtration systems inspired by natural processes.

BP 14.14 Tue 10:00 P3

Autonomous, intrinsic circadian oscillator at cell membranes — •Mauro Ariel Forlino[1], Oreste Piro[2], and Martín García[1] — [1]Universität Kassel, Kassel, Germany — [2]Universtat de les Illes Balears, Palma, España

Circadian rhythms originated in endogenous cellular clockworks are the evolutionary solution that allows organisms to anticipate and synchronize their internal processes with the predictable changes in their environment on a daily basis. According to the conventional paradigm, eukaryotic cells generate circadian rhythms as outputs from gene-based biochemical oscillators comprised of transcription/translation feedback loops, necessarily involving processes occurring within the nucleus. However, mounting evidence has recently emerged indicating that circadian rhythms also exist in cells devoid of such nuclear clocks, notably seen in the circadian variation of red blood cell metabolism. Here, we demonstrate the existence of a completely different mechanism for generating endogenous circadian oscillations that solely involves processes within the cell membrane and its immediate vicinity, entirely independent of the nuclear clock. Rather than relying on the transcription/translation/repression loop as in nuclear oscillators, this membrane-located clock operates through an analogous regulatory circuit that involves the homeostatic regulation of ion channels and their gating kinetics.

BP 14.15 Tue 10:00 P3

Influence of the sapogenin gypsogenin on vesicles from 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) — •Melanie Gettinger and Thomas Hellweg — Physical & Biophysical Chemistry, University Bielefeld, Bielefeld, Germany

Small unilamellar vesicles (SUVs) composed of phospholipids, such as 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC), are commonly used as model membrane systems. DMPC bilayers undergo phase transitions from a gel to a fluid phase at around 24°C. While the effects of saponins on DMPC membranes are well-documented, the impact of their aglycones, sapogenins, remains less explored. Gypsogenin, a pentacyclic triterpenoid found in soapwort (Saponaria officinalis) and gypsum herb (Gypsophila oldhamiana), is of interest due to its anti-cancer potential. Gypsogenin shares structural features with cholesterol but has contrasting effects on membrane properties. While cholesterol increases membrane thickness and reduces fluidity, gypsogenin incorporation decreases the vesicle core radius and membrane thickness, as shown by small-angle X-ray scattering (SAXS) and cryo-TEM. UV-vis spectroscopy was used to monitor turbidity in solutions containing 0 to 25 mol% gypsogenin over a wide temperature range, showing a reversible increase upon cooling, indicating thermally reversible phase transitions. SAXS measurements revealed significant structural changes at 25 mol%. The core radius and membrane thickness decreased compared to pure DMPC vesicles. These findings suggest that gypsogenin alters DMPC membranes significantly at higher concentrations.

BP 14.16 Tue 10:00 P3

Properties of Long-Chain Lipid Enriched Regions in Biological Membranes: Insights from MD Simulations — •Annemarie Quas, Clara Rickhoff, and Andreas Heuer — Institut für Physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster

Experimental studies of yeast plasma membranes reveal gel domains enriched in long-chain lipids and depleted in ergosterol [1]. To explore these findings, we perform coarse-grained molecular dynamics simulations of membranes with varying concentration of long-chain lipids. To enhance our understanding, we simulate both asymmetric membranes with long-chain lipids in the outer leaflet, as observed experimentally, and symmetric membranes containing long-chain lipids in both leaflets. Our analysis focuses on characterizing key membrane properties and examining the influence of long-chain lipids. The role of ergosterol is also investigated. Additionally, we assess non-affine lipid movements to provide insights into the dynamics within these gel domains. This study aims to bridge experimental observations with molecular-level mechanisms, advancing our understanding of gel-phase organization and its implications for membrane functionality.

[1] Aresta-Branco *et al.*, *J. Biol. Chem.* **2011**, 7, 5043-5054

BP 14.17 Tue 10:00 P3

G-FETs for label-free biosensing of protein interactions — •Florian Steinbach, Mykola Fomin, Margarete Schwirblat, and Carola Meyer — Institute of Physics, University of Osnabrück, Germany

Graphene field-effect transistors (G-FETs) offer a promising approach for label-free biosensing due to their sensitivity and compatibility with liquid environments. In this work, we investigate liquid-gated G-FETs functionalized with lipid monolayers for detecting protein interactions at membrane interfaces.

The fabrication process was refined to improve device stability and reduce measurement variability. To enable reusability, we employed tris-NTA-functionalized lipids, allowing reversible binding and elution of hexahistidine (H6)-tagged proteins while preserving device functionality for subsequent detection cycles. Adjustments to the functionalization protocol included histidine-based elution, which better preserved the passivation layer compared to standard imidazole methods. Electrical measurements were used to monitor functionalization steps and protein interactions. Using monomeric enhanced green fluorescent protein (H6-mEGFP) as a model system, we present characteristic shifts and changes in transconductance during each step of the protocol.

These developments contribute to the optimization of G-FETs for biosensing applications, with particular attention to the stability of functionalized interfaces under physiological conditions. The findings will be discussed in the context of improving sensor design and extending the approach to more complex biomolecular systems.

BP 14.18 Tue 10:00 P3

Theory of spatial aggregation and shell formation — •Pranay Jaiswal, Ivar Haugerud, and Christoph Weber — Institute of Physics, University of Augsburg, Augsburg, Germany

Many biological systems use coexisting phases composed of proteins and RNA to regulate chemical processes and molecular transport. In particular, the interface can act as a nucleation site for aggregation of proteins, leading to the formation of a solid-like shell. This shell provides a physical barrier for molecular transport of further biomolecules, giving rise to molecule-specific interface permeabilities. Here we propose a theoretical model for spatio-temporal protein aggregation in phase-separated systems. To this end, we use a phase-field of proteins and RNA combined with a phase-field characterising the solid-like, aggregated state. Our key finding is that aggregation is thermodynamically favored at the interface, making aggregation shells a likely phenomenon in phase-separated systems of aggregation-prone proteins. We show how such aggregation shells control molecular transport and shell permeabilities. Our theory can be applied to experimental systems undergoing irreversible aggregation to unravel the molecular mechanism underlying ageing in protein mixtures.

BP 14.19 Tue 10:00 P3

Cell-free protein synthesis measured in flowing nanolitre-droplets — Benno Schedler[1], Alexandros Katranidis[2], and •Jörg Fitter[1,2] — [1]AG Biophysik, I. Physikalsiches Institut (IA), RWTH Aachen University, D-52074 Aachen, Germany — [2]Forschungszentrum Jülich, ER-C-3, D-52425 Jülich, Germany

Cell-size confinement of biological reactions by utilizing microfluidic water-in-oil droplets has been widely used to revolutionize the field of biomolecular research. This approach capitalizes on the precise control and manipulation of nanoliter-sized droplets within microfluidic channels. The confinement facilitates reduced reagent consumption and improved scalability. Analysing cell-free protein synthesis (CFPS) is an ideal application of this approach and represents a complex multistep process which can be monitored in individual droplets if fluorescent proteins are synthesized [1]. Understanding the physicochemical principles underlying CFPS reactions, including the role of macromolecular crowding, is crucial for optimizing protein synthesis yields and functionality [2]. Here we present the results of our ongoing research using the example of the synthesis of green fluorescent protein (GFP), which we have analysed employing confocal fluorescence microscopy. Focus is set on the high throughput capability of the approach and thus the possibility of analysing several hundred parallel reactions. The latter provide important information about the average synthesis productivity and the distribution widths for reactions under different environmental conditions. [1] Hansen et al., 2016, Nature Nanotechnology, 11, 191; [2] Kempf et al., 2017, Scientific Reports, 7, 46753

BP 14.20 Tue 10:00 P3

Enhancing polymerization of prebiotic building blocks by wet-dry cycling — •Almuth Schmid and Dieter Braun — AG Braun, LMU Systems Biophysics, Munich, Germany

Prebiotic chemistry is limited by several factors as concentration or availability of starting materials on the early Earth. On top of that, many artificial and natural activation agents are too complex to have been a part of prebiotic reaction networks. To overcome this problem, amino acids might help reaching ideal environmental conditions, enhancing prebiotic reactions like polymerization of nucleotides. Preliminary experiments demonstrated, that in a wet-dry cycling system rel. yields of GC polymers are boosted up to 70% in the presence of amino acids.

By using wet-dry cycles and including other prebiotic plausible activating agents like volcanic rocks, a better control of the polymerization can be accomplished. Tracking the polymerization on tholeiite basaltic rock with SEM reveals first hints on where and how the polymers interact with the mineral.

BP 14.21 Tue 10:00 P3

Phase-separation enhances sequence selection via templated ligation — •Manav Koul, Ivar Haugerud, and Christoph Weber — Universität Augsburg, Universitätsstraße 2, 86159 Augsburg

The emergence of highly selective catalytic sequences was a crucial step towards the origin of life. templated ligation of RNA has been proposed as a pre-biotic mechanism to achieve self-replicating sequences without complex machinery. A question remains as to how sufficiently long and abundant templates can emerge from short nucleotides in a non-conducive prebiotic pool. As phase separation has been shown to provide versatile hubs of correlated sequences, we investigate its role in facilitating and directing templated ligation. To this end, we develop a non-equilibrium thermodynamic model to describe the oligomerization of sequences and their ligation at non-dilute conditions in phase-separated systems. We find that phase-separation enhances the selection pressure of this mechanism, resulting in a sequence distribution dominated by highly structured sequence of low entropy. Our results highlight that out-of-equilibrium condensed phases could provide versatile hubs for Darwinian-like evolution toward functional sequences, both relevant for the molecular origin of life and de-novo life.

BP 14.22 Tue 10:00 P3

Phase Transitions in Non-Hydrated DPPC Lipid Bilayers Deposited on Silicon: Effects of Dry Nitrogen Atmosphere and Thermal Cycling — •Nicolás Moraga[1], Daniel Saavedra[1], Nancy Gomez-Vierling[1], Marcelo A. Cisternas[2], María José Retamal[3], and Ulrich G. Volkmann[1] — [1]Instituto de Física, Pontificia Universidad Católica de Chile, Santiago, Chile — [2]Escuela de Ingeniería Industrial, Universidad de Valparaíso, Chile — [3]Facultad de Ingeniería, Universidad Finis Terrae, Santiago, Chile

This study investigates the phase behavior of DPPC lipid bilayers in a non-hydrated state, deposited on silicon substrates, under conditions that are both experimentally innovative and highly relevant for applied science and fundamental research. By assembling these bilayers in vacuum and exposing them to dry nitrogen atmospheres, we present a novel platform that extends beyond classical hydrated systems, with significant implications for biosensing technologies. Through controlled thermal cycling using high-resolution ellipsometry, a technique offering exceptional sensitivity to subtle changes, we analyze phase transitions, uncovering the impact of hydration-free environments on lipid bilayer organization. These findings provide new insights into the thermal resilience of DPPC bilayers, highlighting potential phase stability domains. Additionally, this approach simulates extraterrestrial-like conditions where water is absent, underscoring the adaptability of lipid-based structures and advancing our understanding of molecular organization under vacuum and inert atmospheres. Acknowledgements: ANID Fellowships (NM, DS, NGV); Puente UC 2024-25.

BP 14.23 Tue 10:00 P3

Cooperative Effects in Compartmentalized Irreversible Self-Assembly — •Severin Angerpointner, Richard Swiderski, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Germany

From biomolecular compartments, protein patterns to porous rocks: Many biological and chemical systems like living cells or prebiotic chambers exhibit some form of spatial organization which separates biochemical processes. This is known to play a key role in the assembly of virus capsids or the enrichment of prebiotic chemicals. We systematically explore the effects of such spatial separation on the self-assembly of irreversibly binding identical particles. We show that already in a simplified model of two coupled biochemical compartments cooperative effects emerge through limiting compartment exchange. Further, these findings generalize to spatially extended systems like intracellular chemical gradients or membrane-assisted assembly.

BP 14.24 Tue 10:00 P3

Mathematical modelling of immune response on the example of psoriasis — •Nadezhda Esenkova[1,2], Lukas Pöschl[1,2], Gerard C. L. Wong[3], and Vasily Zaburdaev[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [3]University of California, Los Angeles, USA

In recent years it was shown that antimicrobial peptides (AMPs) can contribute to the immune response by triggering Toll-Like Receptors (TLRs) on immune cells. Apart from natural AMPs it was suggested that proteolytic enzymes, secreted by neutrophils can digest other signaling molecules to AMP-like fragments, which can stimulate immune response and lead to disease progression. The goal of this work is to create a mathematical model of immune response by introducing this novel link of AMP-like fragments. To this aim we constructed a comprehensive signaling network of the immune response based on one of the best studied autoinflammatory diseases – psoriasis. Taking into account the key biological pathways we reduced it to the core network model, which we investigate using theoretical dynamical systems analysis and modern machine learning methods. We aim to understand how the hypothesized mechanism of autoinflammation due to AMP-like fragments augments the disease outcomes from full resolution, to chronification and rapid exacerbation.

BP 14.25 Tue 10:00 P3

Formation of thermally driven pH gradients from salts — •Riccardo Schiroli, Thomas Matreux, and Christof B. Mast — Systems Biophysics, LMU München, Munich, Germany

The impact of pH on biomolecule stability and chemical reactions suggests its crucial role in prebiotic chemistry. Thermophoresis, the movement of molecules along a thermal gradient, has been shown to accumulate and select a wide range of biomolecules, including RNAs and amino acids as well as different salt species leading in specific conditions to the emergence of pH gradients.

In this study, we investigated the formation of heat flow driven pH gradients in simulated rock fissures under various experimental conditions, including different salt solutions, initial pH values, and temperature gradients. Ion chromatography, combined with complexation techniques and fluorescent analysis, was used to analyze the distribution of ions and pH profiles within the fissures.

Our findings show that heat flows can efficiently induce pH gradients in solutions containing various salt species. We observed significant ac-

cumulation of common ions, leading to pH gradients in both alkaline and acidic solutions. Furthermore, we found that certain metal ions, such as lanthanides and iron, can significantly enhance the formation of pH gradients, even at micromolar concentrations. This study provides evidence for the role of heat flows in creating localized pH gradients under prebiotically plausible conditions. Our results highlight the ease with which pH gradients can form under a wide range of prebiotic plausible conditions, driven by simple heat flows.

BP 15: Cell Mechanics I

Time: Tuesday 11:45–13:00 Location: H44

Invited Talk BP 15.1 Tue 11:45 H44

Does Oncology Need Physics of Cancer? — •Josef Käs — Peter Debye Institute for Soft Matter Physics, Leipzig University, Linnéstr 5, 04103 Leipzig

Cancer is a complex disease that accounts for nearly one in six deaths worldwide. More than 90 percent of deaths are due to metastasis * the process by which cancer cells spread from the primary tumor and seed a secondary tumor in a distant tissue. Despite advances in cancer treatment, metastatic recurrences remain a significant challenge. Understanding metastasis is crucial for a reliable predictive diagnosis needed for personalized oncology and to develop therapies that inhibit cancer spreading. The metastatic cascade routes in a mechanical problem for tumor cells on their way through the human body squeezing through dense tissues. Two clinical trials with more than 2000 breast cancer patients in each study prove that the onset of cancer cell motility can be explained as an unjamming transition and local cancer spreading of cancer cell clusters embedded in ECM must be described as active nematic droplets in a nematic phase. The gained physical parameters can be used a prognostic tumor marker for metastatic risk that improves breast cancer diagnosis by 26 percent. Beyond diagnostics the mechanical modulation of cancer cells by adipocytes points us towards migrastatic therapies to suppress metastasis.

BP 15.2 Tue 12:15 H44

Prostate cancer associated fibroblasts have distinct morpho-mechanical features that predict patient outcome — Antje Garside[1], Angela Jacobi[1], Shivakumar Keerthikumar[2,3], Michelle Richards[2], Birunthi Niranjan[2], Gail Risbridger[2,3], Mitchell Lawrence[2,3], and •Anna Taubenberger[1] — [1]BIOTEC, TUD, Dresden, Germany. — [2]Monash University, Victoria, Australia — [3]Peter MacCallum Cancer Centre, Melbourne, Australia.

Prostate cancer is among the most commonly diagnosed types of cancer. A key role in tumor progression has been attributed to the tumor stroma including its cellular components such as cancer associated fibroblasts (CAFs). Here we present a comprehensive study where we quantitatively assessed the morpho-mechanical properties of patient-derived prostatic CAFs and matched normal prostatic fibroblasts from a cohort of 35 patients, through combination of cell morphometric analysis and high-throughput mechanical probing of single cells by real-time deformability cytometry. CAFs comprised distinct morpho-mechanical features compared to their normal counterparts, including nuclear size and shape, cytoskeletal arrangement, cellular volumes and elastic properties. A combined score of these mechanical and morphological parameters distinguished patients with shorter and longer time to clinical relapse. Morpho-mechanical changes across patients were correlated with transcriptomic alterations in cellular components and pathways. In summary, our results suggest that high-throughput assessments of the biophysical properties of CAFs can serve as a complementary tool to predict patient outcome.

BP 15.3 Tue 12:30 H44

Viscoelasticity of Cancer Cells: New Insights from Magnetic Rotational Spectroscopy — •Jean-François Berret — Université Paris Cité, CNRS, Matière et systèmes complexes, 75013 Paris, France

Cell mechanical properties are linked to tumor progression and can serve as diagnostic biomarkers. Over the past two decades, numerous studies have shown that cancer cells are softer than healthy cells. While the viscoelastic nature of cells is well known, most studies focus on elasticity, with limited attention to viscosity. To address this, we developed Magnetic Rotational Spectroscopy (MRS), an active technique using non-toxic magnetic wires embedded in the cytoplasm and tracked via optical microscopy under a rotating magnetic field. This allows simultaneous measurement of viscosity η and elastic modulus G. MRS studies on 15 human and animal cell lines, both healthy and cancerous, uncovered a new finding: intracellular viscosity increases with wire size following a quadratic η(L)-relationship. Furthermore, in breast epithelial cells, only viscosity, not elasticity, could differentiate cells with low and high metastatic potential. A meta-analysis of literature on cell viscosity, covering whole-cell and intracellular data finally reveals that cancer cells have viscosities about 50% lower than healthy cells, suggesting that cancer cells are not only softer but also more fluid, offering potential for selective diagnostic tools in cell biomechanics. [1] A.M. Markl et al., Cancer Heterog. Plast., (2024). [2] J.-F. Berret, Nat. Commun. 7, 10134 (2016). [3] M. Dessard et al., Nanoscale Adv. 6, 1727 (2024).

BP 15.4 Tue 12:45 H44

Living Cells Feel the Surface Tension of Soft Solids — •Johannes Rheinlaender, Hendrik von Eysmondt, and Tilman E. Schäffer — Institute of Applied Physics, University Tübingen, Germany

For about 20 years it has been known that living cells actively respond to the stiffness of their microenvironment - most obviously - by a change in cell spreading area but also other properties such as stiffness, nucleus shape, and gene expression, denoted as mechanosensing. These effects are commonly investigated using hydrogels with a bulk Young's modulus in the kPa range, where cells respond to substrate stiffnesses typically between 1 and 100 kPa. On other soft materials such as elastomers, cell behavior has been shown to be different and weaker, plateauing below about 10 kPa, but the reason remained a matter of debate. On the microscale, surface properties such as surface tension are of increasing relevance, but probing interfaces with micro-indentation techniques such as atomic force microscopy is challenging due to adhesion effects. We therefore use scanning ion conductance microscopy (SICM), a unique scanning probe method benefiting from its non-contact measurement principle, to probe the surface tension of soft solids showing that elastomers exhibit surface tensions of about 10 mN/m, relatively independent of their bulk Young's modulus and surface treatment. Hence, cells mostly "feel" the bulk properties of elastomers for Young's moduli above about 10 kPa, but below mostly the surface tension, demonstrating that the substrate's surface tension is an important yet underestimated aspect in mechanobiology.

BP 16: Focus Session: Nonlinear Dynamics in Biological Systems II (joint session DY/BP)

Nonlinear dynamics play a central role for biological systems to achieve remarkable complexity and adaptability. They underlie processes where small changes cascade into large effects, critical thresholds drive transitions, and feedback mechanisms maintain intricate balances. Biological systems are often far from equilibrium, exhibiting behaviors shaped by competing forces, stochastic fluctuations and emergent behavior. From the amplification of sensory signals near bifurcation points to the development of turbulence, concepts from nonlinear dynamics provide a unifying framework for studying patterns, stability, and collective behavior in living systems. This focus session explores the richness of nonlinear dynamics across biological scales, from molecular circuits to population-level phenomena, spanning vastly different fields from cardiac dynamics, embryogenesis and cell motility to active fluids, condensates and origin of life. Through theoretical models, experimental insights, and computational approaches, the talks illustrate how nonlinear-dynamics principles unravel the mechanisms driving function and complexity in biology, offering new perspectives across disciplines.

Organized by Philip Bittihn (Göttingen), Stefan Klumpp (Göttingen), and Carsten Beta (Potsdam)

Time: Tuesday 14:00–15:15 Location: H43

Invited Talk BP 16.1 Tue 14:00 H43

Mechanistic origins of temperature scaling in the early embryonic cell cycle — •Lendert Gelens — Laboratory of Dynamics in Biological Systems, Department of Cellular and Molecular Medicine, KU Leuven, Herestraat, 49, Leuven, Belgium

Temperature profoundly impacts organismal physiology and ecological dynamics, particularly affecting ectothermic species and making them especially vulnerable to climate shifts. Even though complex physiological processes usually involve dozens of enzymes, empirically it is found that the rates of these processes often obey the Arrhenius equation, which was originally derived for single enzyme-catalyzed reactions. Here we have examined the temperature scaling of the early embryonic cell cycle, with the goal of understanding why the Arrhenius equation approximately holds, and why it breaks down at temperature extremes.

Using experimental data from different frog, fish, fly, and worm species, we find that the apparent activation energies for the early embryonic cell cycle for diverse ectotherms are all similar. Computational modeling and experiments with frog egg extracts show that the non-Arrhenius scaling can be accounted for by biphasic temperature scaling in critical individual components of the cell cycle oscillator circuit, in combination with imbalances in the activation energies for different partially rate-determining enzymes. These findings provide mechanistic insights into the dynamic interplay between temperature and complex biochemical processes, and into why biological systems fail at extreme temperatures.

BP 16.2 Tue 14:30 H43

Reshaping morphogen gradients through porous tissue architecture — •Diana Khoromskaia[1,2] and Zena Hadjivasiliou[1,2,3] — [1]Francis Crick Institute, London, United Kingdom — [2]University College London, London, United Kingdom — [3]London Centre for Nanotechnology, London, United Kingdom

The morphogenesis of tissues during embryonic development is controlled by concentration gradients of morphogens – signalling molecules whose readout determines cell fate decisions. How the spread of morphogens is affected in tissues with complex geometry and spatially heterogeneous architecture is not well understood. To address this question, we introduce a porous vertex model, by explicitly considering the network of extracellular spaces between the cells. Morphogens produced by source cells disperse through the tissue via three modes of transport: extracellular diffusion, membrane-bound diffusion, and cell-based transport through recycling. With this model we investigate numerically and analytically how cell-scale geometry, such as cell size, cell shape anisotropy, and cell distance, influences effective diffusion and degradation of morphogens at tissue-scale. We further show that a non-linear coupling between cell packing and morphogen concentration renders the morphogen gradient robust to perturbations, for instance by locally buffering fluctuations in the production. Our characterisation of tissues as active porous materials provides new insights into how morphogenesis and cell fate determination may interact during embryonic development.

BP 16.3 Tue 14:45 H43

Active viscoelastic condensates provide controllable mechanical anchor points — •Oliver Paulin[1], Luise Zieger[2,3], Júlia Garcia-Baucells[5], Alexander Dammermann[5], Sebastian Aland[2,3,4], and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [2]TU Bergakademie Freiberg — [3]HTW Dresden — [4]Center for Systems Biology, Dresden — [5]Max Perutz Labs, University of Vienna

Many biological materials must couple mechanical strength with the ability to rapidly self-assemble at a specific location. In particular, biomolecular condensates readily self-assemble via phase separation, but may also need to anchor external forces to fulfil their function. Spatial localisation of condensate formation can be controlled by active cores that preferentially drive the production of condensate material at a particular point, while resistance to external forces can be facilitated by viscoelastic material properties. Here, we develop a continuum model of viscoelastic growth around an active core, and investigate the results in a spherically symmetric geometry. We find that viscoelastic stresses restrict condensate growth, but also impart resistance to deformation. We investigate the effect of varying different mechanical properties on condensate growth and strength, and also study how strain-dependent material incorporation may limit the maximum rate of growth. Finally, we compare the predictions of our model to experimental data from centrosomes in C. elegans embryos, identifying a parameter regime in which rapid growth can be combined with appropriate mechanical strength.

BP 16.4 Tue 15:00 H43

Modelling cell crawling on different substrate stiffness — Sohei Nakamura and •Mitsusuke Tarama — Kyushu University, Fukuoka, Japan

Crawling cells sense the mechanical properties of the underlying substrate and change their dynamics accordingly. This ability called durotaxis is of great importance in various biological processes including development and homeostasis. In order to understand how intracellular chemical reactions and cellular mechanics give rise to durotaxis, we constructed a simple model from reaction diffusion equations for intracellular chemical compounds and force balance equations for the intracellular mechanics including the effect of the substrate stiffness. We found that within the model, the cell speed and diffusion coefficient change non-monotonically with the substrate stiffness, indicating the existence of an optimal substrate stiffness for migration. This non-monotonic behavior of the cell speed is consistent with experimental observations and can be understood to be caused by the competition between substrate adhesion and cell shape deformation. We further discuss cell migration on a patterned substrate.

BP 17: Poster Session II

Active matter, bioimaging, biomaterials and biopolymers, cell mechanics, cytoskeleton, protein structure and dynamics, single-molecule biophysics, statistical physics of biological systems, tissue mechanics, nonlinear dynamics in biological systems

Time: Tuesday 18:00–20:30 Location: P4

BP 17.1 Tue 18:00 P4

Effect of cilia length on the motility of confined microbes — •Tom Sosniok, Alexandros Fragkopoulos, Rodrigo Catalan, and Oliver Bäumchen — University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany

Many microorganisms utilize their cilia or flagella to propel and navigate through their surrounding liquid environment. Often times though, the habitats of such microswimmers comprise confined spaces, and therefore, cell interactions with boundaries play an important role on their navigation. *Chlamydomonas reinhardtii*, a biciliated, green microalga that is commonly found in soil, typically swims in close proximity to curved boundaries [1]. We found that this near-wall swimming motility is controlled by gradients of wall curvature and steric interactions between the cilia and the surface [2]. Here we explore the effect of the cilia length on the motility and surface interactions of the cells using different *C. reinhardtii* mutant strains with different cilia lengths in quasi-2D circular confinement. We extract information about their motion from their mean squared displacements and visualize the wall-guided swimming via relative and radial probability densities. By comparing the results for the different strains we can directly analyse the influence of the cilia length on their swimming motility in confinement.

[1] T. Ostapenko, et al., *Phys. Rev. Lett.* **120**, 068002 (2018).
[2] J. Cammann et al., *Proc. Natl. Acad. Sci. U.S.A.* **118**, e2024752118 (2021).

BP 17.2 Tue 18:00 P4

Stochastic modeling of a two-component polymer engine — •Yasmin Abdelghaffar[1] and Marcus Jahnel[1,2] — [1]Cluster of Excellence Physics of Life, Technical University Dresden, Dresden, Germany — [2]Biotec, Technical University Dresden, Dresden, Germany

Long coiled-coil tethering proteins and small GTPases have recently been shown to form a new class of biomolecular motors driven by entropic collapse. The working principle of this motor is a cyclic flexibility transition of its filamentous tether, triggered by the GTPase unit. While a basic working model was proposed (Singh, 2023), many fundamental aspects of these two-component molecular motors remain unexplored. Here, we developed a stochastic model as an over-damped to-state semi-flexible polymer to describe the mechanochemical cycle that drives this motor. Using this model, we can predict how efficiency and power of this motor are affected by changes in model parameters such as persistence lengths. Additionally, by introducing force-dependent rates in the mechanochemical coupling of our model, we can potentially explain previous discrepancies in the measured hydrolysis rate of GTP between in bulk experiments, which occur under no force, and tweezer experiments, where the system is under tension. Our simulation study thus makes an indication on the chemical nature of the coiled-coil protein within the motor, identifying it as a potential GTPase-activating protein.

BP 17.3 Tue 18:00 P4

Modeling dynamics and density distribution of magnetotactic bacteria in traps — •Theo Richter, Sascha Lambert, and Stefan Klumpp — Institut für Dynamik komplexer Systeme, Universität Göttingen, Göttingen, Germany

Magnetotactic bacteria are microorganisms that navigate using internal magnetosomes, aligning them along magnetic fields. They represent an intriguing model system for studying active Brownian particle dynamics under an external alignment field. Previous studies have analyzed their movement through crowded channels, where the orientation along the magnetic field and their interaction with obstacles prove to be important mechanisms for navigation. In such complex environments, bacteria often find themselves trapped in corners, where the dynamics of how they escape these traps are crucial and remain mostly unexplored.

In this work, we aim to understand the density profiles, escape rate and general dynamics of single active Brownian particles under an alignment field inside trapping geometries. We investigate these quantities via simulations in varying trap geometries, with a focus on triangular traps, characterizing the effects of system parameters such as magnetic field strength and particle-wall interactions. We relate the behavior of the bacteria in these geometries to the sedimentation of active Brownian particles.

BP 17.4 Tue 18:00 P4

Light-switchable adhesion and clustering of *C. noctigama* at liquid-air interfaces — •Gustav Nolte, Alexandros Fragkopoulos, and Oliver Bäumchen — University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany

Microalgae are unicellular photoactive organisms that are ubiquitous in liquid-infused natural environments. The biciliated microalga *Chlamydomonas reinhardtii* shows light-switchable adhesion and clustering at surfaces, a process so far exclusively observed for solid-liquid interfaces [1,2,3]. Here we report on the light-switchable formation of clusters by *Chlamydomonas noctigama*, a related species with increasing relevance in the field of optogenetics, at liquid-air interfaces. The morphology and dynamics of these clusters differ significantly from the clusters formed by *C. reinhardtii*. Apart from the average cluster size and polydispersity, the growth dynamics of individual clusters are studied for a wide range of cell densities. We find a critical cell density above which the number of clusters decreases over time. For the underlying principles of cluster formation and dynamics, we address potential mechanisms like preferential attachment and Ostwald ripening. Reversible clustering may provide an advantage for *C. noctigama* by allowing the cells to accumulate in locations optimal for photosynthesis while also increasing resilience to environmental stress within the cluster.

[1] S. Till, et al., *Phy. Rev. Res.* **4**, L042046 (2022).
[2] R. E. Catalán, et al., *Soft Matter* **19**, 306 (2023).
[3] C. T. Kreis, et al., *Nat. Phys.* **14**, 45 (2018).

BP 17.5 Tue 18:00 P4

The Dynamics of Spatiotemporal Self-organization in Active Turbulence — •Henri Jörn Schmidt — Max-Planck institute for self-organisation and dynamics, Göttingen, Germany

Spontaneous pattern formation in nature has been subject to extensive research in recent decades, with more and more emphasis being put on the dynamics of their creation processes.

In this work we investigate coherent structures in fluid flows. Specifically, this work concentrates on eddy currents found in the turbulent regime of active nematics. We analyse their formation and evolution as well as how their dynamics is affected by the cross-talk between different length scales. In doing so, we introduce a new methodology to record the overlaps of eluded structures in an agent-based approach. This allows for size changes in individual structures without inflicting biases in the computed intersection ratios.

Our results seem to indicate no particular cascade of different length scales. However, we do observe an universal evolution of the eddy currents, marked by a pronounced growing and shrinking phase. Usually, these stages take place within an encapsulating parent structure. Likewise, as the eddies have attained their nominal size, they give rise to new eluded structures themselves. These dynamics seem to be independent from both, the size ratio of clusters and their elapsed life time.

BP 17.6 Tue 18:00 P4

Macroscopic transports in cellular aggregates driven by dipole forces — •Subhadip Chakraborti[1,2] and Vasily Zaburdaev[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

The large-scale collective behavior of biological systems can be understood through macroscopic transport processes that emerge from the active interactions of individual components at the microscopic level. A striking example is the clustering and the associated transport slowdown observed in colonies of *Neisseria gonorrhoeae* bacteria, driven by active, contractile forces mediated by pili. In this study, we analytically

derive the fluctuating hydrodynamics from the microscopic dynamics of a 2D model system representing an *N. gonorrhoeae* bacterial colony. The hydrodynamic current of cells involves two macroscopic transport coefficients: bulk diffusivity and conductivity, which generally depend on cell density and other microscopic parameters. Remarkably, our simulation results strongly support the analytical predictions of transport slowdown during the colony formation process. Beyond bacterial colonies, these findings offer insights into how contractile forces influence transport in other biological systems, such as tumor spheroids and neuronal organoids, and suggest experimental approaches for studying these phenomena.

BP 17.7 Tue 18:00 P4

Dynamics, stresses and cell fate in confluent cell monolayers — •Stefano Villa[1,2], Giorgio Scita[3], Roberto Cerbino[4], and Fabio Giavazzi[2] — [1]Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen — [2]Universitá degli Studi di Milano, 20090 Segrate — [3]IFOM-FIRC Institute of Molecular Oncology, 20139 Milan — [4]University of Vienna, 1090 Vienna

Confluent cell monolayers are 2D active systems exhibiting a variety of dynamical states, ranging from solid-like jammed systems to fluid-like flocking systems. Such a rich panorama results in different mechanical stresses the single cells within the monolayer are subjected to. Due to their impressive complexity, cells do not merely react to the mechanical stresses but actively interact with the environment, e.g. adapting their mechanical properties to the stimuli. The investigation of the close interplay between dynamical state and mechanical properties of tissues is therefore of paramount interest for unraveling how cells respond to mechano-physical stimuli. We present a detailed analysis based on cell segmentation performed on time-lapse microscopy videos showing the effect of motility-induced stresses on the single cell mechanics, comparing cell models mimicking healthy tissues and tumor-like tissues. We show how the increase in dynamics leads to larger cell deformations to which the cells respond by increasing the stiffness of the nucleus. Finally, we show how mechanical stresses within the monolayer can affect tissue morphogenesis in real systems, thus highlighting once again the relevance of mechano-physical stimuli for the cell and tissue development and fate.

BP 17.8 Tue 18:00 P4

Analysis of Wall-Torques for Rod-Shaped Active Particles — •Merle Duchêne, Sascha Lambert, and Stefan Klumpp — University of Göttingen, Institute for the Dynamics of Complex Systems, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The motility of living things and synthetic self-propelled objects is often described using Active Brownian particle models. To account for interactions with complex environments, this model can be expanded with empirical forces or torques, such as those describing their alignment with an obstacle or wall after a collision. Here, we evaluate the quality of these empirical models by comparing their output predictions with trajectories of rigid rod-shaped active particles that scatter sterically at a flat wall. Specifically, we analyze the torque reorienting the rod-shaped particle and compare it to predictions from a phenomenological model. We employ a classical least-squares method to evaluate the instantaneous torque and identify essential model parameters. In addition, a Bayesian inference procedure can be applied to construct the posterior distribution of plausible model parameters which provides a complementary perspective to the least-squares analysis.

BP 17.9 Tue 18:00 P4

Onset of bioconvection in a simple continuum model — •Marius M. Kaiser, Fabián Álvarez-Garrido, and Michael Wilczek — Universität Bayreuth

Dense suspensions of swimming micro-organisms show bioconvection, i.e.˜the emergence of self-organized flow patterns much larger than the individual swimmers, under certain conditions. Here, we analyze the onset of bioconvection in a simple continuum model. The model is derived from the Fokker-Planck equation for the swimmer concentration field and the swimmer orientation field [Pedley, J. Fluid. Mech. 647, 335 (2010)] coupled to the Navier-Stokes equation, in which we only consider buoyancy effects (no cell stresses) and approximate higher-order moments in terms of the polar order parameter. A linear stability analysis in the idealized case of a prescribed polar orientation field shows that the system exhibits a type-II instability. The results of our linear stability analysis are in agreement with direct numerical simulations of our model. Simulations of the model, now with dynamically evolving polar orientation field, suggest that the type of spatial instability remains the same, albeit with shifted critical values. Our findings shed light on the mechanism driving pattern formation in this type of suspensions.

BP 17.10 Tue 18:00 P4

DNA origami laden with bespoke magnetic nanocubes: A route to programmable torques at the nanoscale — Florian Rothfischer[1], Yihao Wang[2], Lennart Weiss[1], Christopher Pauer[3], Kevin Lang[3], Susanne Kempter[3], Rabia Amin[2], Elena Eiwanger[3], Jan Lipfert[4], Tim Liedl[3], Friedrich C Simmel[1], Joe Tavacoli[3], and •Aidin Lak[2] — [1]Physics Department E14, Technical University Munich — [2]Institute for Electrical Measurement Science and Fundamental Electrical Engineering and Laboratory for Emerging Nanometrology (LENA), TU Braunschweig — [3]Faculty of Physics and Center for NanoScience, LMU Munich — [4]Institute for Physics, Augsburg University

Magnetic-field responsive actuators offer minimally-invasive and deep-tissue perturbation of cellular processes. Despite progress, the magnetic manipulation of cells at the single receptor level is still challenging; magnetic nanoparticles (MNPs) can only exert ˜ fN forces. To achieve biologically relevant pN forces, it is necessary to assemble MNPs together in a controllable manner. This has not yet been achieved utilizing soft-synthetic templates, where control over the number, and orientation of MNPs remains a challenge. DNA origami (DNAO) can overcome this limit, specifically so for its capacity to arrange nanoparticles at high spatial resolution. Here, we demonstrate assembly of bespoke MNPs on 6 helix-bundle DNAO and show the controlled magnetic rotation of magnetic DNAOs under circulating magnetic fields of 8 mT. Our magnetic DNAOs are promising torque nanoprobes for activation of sub-cellular processes at high resolution.

BP 17.11 Tue 18:00 P4

Engineering Shear-Thinning Hydrogels: A Dynamic Scaffold for 3D Tissue Culture — •Bruno Schmelz[1], Fen Li[2], Kai Zhang[2], and Timo Betz[1] — [1]Third Institute of Physics, University of Göttingen, Germany — [2]Sustainable Materials and Chemistry, Department of Wood Technology and Wood-based Composites, University of Göttingen, Germany

Extracellular matrix (ECM) scaffolds are essential for advanced 3D cell culture systems, providing structures for cell movement as well as physical and chemical cues that promote migration, proliferation, and differentiation. Hence, the ECM is crucial for functional tissue formation. However, natural ECM materials used in vitro, such as collagen and elastin, are difficult to control regarding elastic properties, polymer mesh size, and homogeneity. Our objective is to design a dynamic hydrogel tailored to meet the specific requirements of 3D tissue culture, such as viscoelastic properties and cell-binding sites, that initially supports tissue formation but can be dissolved and replaced by cell-generated ECM. We propose a hydrogel with non-covalent cross-linking moieties that allow for reorganization by embedded cells, similar to the reorganization of collagen fibers in physiological tissues. We present the rheological properties of the hydrogels and the initial findings of cell invasion into them. When subjected to stress, the hydrogels exhibit a transition to a more liquid-like state, with the potential to solidify again upon stress relaxation. This behavior allows cells to remodel their surrounding matrix and shape their environment, as evidenced by experiments with cells cultured on the hydrogels.

BP 17.12 Tue 18:00 P4

Supramolecular ordering in lipopolymer monolayers at the air/water interface — •Issam Assi, Heiko Ahrens, and Christiane A. Helm — Institute of Physics, University of Greifswald

Lipopolymers with covalently bound poly(ethylene oxide) (EO_N) bound to the head groups have been introduced to stabilize bilayer membranes. Langmuir monolayers of the lipopolymer DSPE-EO_N at the air/water interface show in the isotherm a transition from the liquid expanded to the liquid condensed phase, which is confirmed by in-situ Grazing Incidence X-ray Diffraction (GID at DESY, Hamburg). A laterally inhomogeneous film of condensed ordered alkyl chains embedded in a matrix of solvated polymers is formed. Small Angle GID shows these lipid domains are ordered in a hexagonal lattice (repeat distance about 12 nm). The films stay homogeneous on the micrometer scale as observed with Brewster Angle Microscopy. On transferred monolayers, these supramolecular phases were observed with AFM. Fast compression of DSPE-EO_{44} monolayers is necessary to maintain the hexagonal superstructure at relatively high lateral pressures, whereas slow

compression induces a lamellar structure. Also, the superstructure of lipopolymers with shorter polymers (DSPE-EO_{11} and DSPE-EO_{22}) was explored.

BP 17.13 Tue 18:00 P4

Nanoscale drug delivery system aggregates controlably on graphite — •Henrik Siboni[1,2], Leonhard Grill[2], and Andreas Zimmer[1] — [1]Pharmaceutical Technology & Biopharmacy, University of Graz, Austria — [2]Single Molecule Chemistry, University of Graz, Austria

Nanoscale drug delivery systems are nanoparticles used to enhance the efficacy of drugs and their effectiveness depends on physical properties such as size, shape and aggregation behaviour. These parameters can be measured on a substrate with atomic force microscopy, but conserving the individual nanoparticles has proven challenging. In this study, we show that the substrate highly-oriented pyrolytic graphite allows for controllable imaging of single as well as aggregated protamine-oligonucleotide drug delivery systems. This approach can potentially be used to screen drug delivery systems and avoid unnecessary in vivo test.

BP 17.14 Tue 18:00 P4

Printed biometamaterials for mechanical regulation of cells — •Clara Schaefer[1], Alexander Berkes[2], Martin Wegener[2], Natalie Munding[1], and Motomu Tanaka[1,3] — [1]Institute of Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany — [2]Institute of Applied Physics, KIT, 76131 Karlsruhe, Gemany — [3]Kyoto University, Kyoto 606-8501, Japan

Ample evidence has shown that cells detect and respond to the mechanical properties of their microenvironment. Materials with non-conventional mechanical properties (mechanical metamaterials) have shown significant effects on human mesenchymal stem cells (Munding, et al. Adv. Funct. Mater. 2024). The key requirements are to make the unit cell size smaller than the cells and to make the materials deformable by cell traction forces. The anisotropic elastic properties lead to different responses in the traction force field that are distinct from those to bulk materials. To deal with multicellular systems and to follow cell migration, one of the challenges is to increase the lateral size to several hundreds of μm. To achieve this goal, we increased the printing speed by using a new multi-focus device in two-photon laser printing. This enables to fabricate even asymmetric metamaterial structures that can potentially be used to induce cell polarization.

BP 17.15 Tue 18:00 P4

Subcellular distribution of green-emitting carbon nanodots — •Mariell Gassen, Mine Polat, Carla Sprengel, and Thomas Heinzel — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Carbon nanodots are promising fluorescent nanoparticles for biomedical imaging applications and drug delivery. They frequently show fluorescence in the blue range, which causes interference with the autofluorescence of the cell [1]. To circumvent this, we produced green-emitting carbon nanodots and incubated them in cells. We report tests about their subcellular distribution and studies of their suitability as carriers for active substances.

[1] S. Fasbender et al. The Low Toxicity of Graphene Quantum Dots is Reflected by Marginal Gene Expression Changes of Primary Human Hematopoietic Stem Cells. Sci Rep 9, 12028 (2019).

BP 17.16 Tue 18:00 P4

Red Blood Cells under brightfield microscopy — •Aaron Kreis, Sarah Tabea Hermes, Thomas John, and Christian Wagner — Experimental Physics, University Saarland

The observation of red blood cells under a conventional light microscope is a common practice in research and medicine. In many cases, the particular cell shape is the object of interest, see [1]. Red blood cells are composed mostly of hemoglobin, which shows its maximum absorption at $\sim$ 420 nm. Nevertheless, the cells are mostly observed under white or red light. Furthermore, the refractive index of the cytosol is greater than that of water and refraction occurs. The combination of refraction and absorption leads to very different microscopy images at different focal points. We have quantified this using calculations by ray tracing and we can explain the observed microscopy images, including the white 'halos' due to refraction at various focal positions. Diffraction isn't a major contribution in observed cell shapes. We demonstrate that the use of blue light results in a significantly better image contrast of the cell shapes without artifacts, compared to the usual observation with white light.

[1] Yoon at. al., Flickering Analysis of Erythrocyte Mechanical Properties, Biophysical Journal 97, 1606, (2009)

BP 17.17 Tue 18:00 P4

High-resolution chemical characterization of retinal pigment epithelium (RPE) using mid-infrared photo-induced force microscopy — •Maryam Ali[1,2], Robin Schneider[1], Patrick Then[1], Mohammad Soltaninezhad[1,2], Sebastian Unger[1,2], Christoph Krafft[1,2], Christine A. Curcio[3], Rainer Heintzmann[1,2], Thomas Ach[4], and Daniela Täuber[1,2] — [1]Leibniz Institute of Photonic Technology, Jena, Germany — [2]Friedrich Schiller University, Jena, Germany — [3]University of Alabama at Birmingham, United States — [4]University Hospital Bonn, Germany

Nanoscale infrared (IR) spectroscopic imaging methods fill a gap in bioimaging. Mid-IR photo-induced force microscopy (PiF-IR) combines powerful IR illumination with non-contact atomic force microscopy, resulting in high spectral and unprecedented spatial resolution ($<$ 5 nm)[1]. We applied PiF-IR to a cross-section of the retinal pigment epithelium (RPE) layer of a human donor eye. The strongly polar RPE cells play a major role in the vision cycle. Several types of autofluorescent granules in RPE cells[2] contribute to fundus autofluorescence, a clinical imaging technique used for the diagnosis of retinal diseases. In spite of their importance, the chemical composition of these organelles is not fully known. A combined chemometrics analysis of three PiF-IR hyperspectra from locations across the RPE layer reveals variations in the protein content of the surfaces of granular organelles. –[1] J. Joseph et al., Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 2024, 306, 123612. [2] K. Bermond et al., IOVS 2020, 61, 35.

BP 17.18 Tue 18:00 P4

Preparation of green fluorescent carbon nanoparticles — •Mine Polat, Carla Sprengel, and Thomas Heinzel — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Carbon nanodots (CNDs) are promising materials for biomedical applications due to their unique fluorescent properties and biocompatible structure. However, many CNDs emit in the blue range, which is less favorable for specific applications. In this project, green-emitting CNDs were synthesized, their optical properties were analyzed, and the quantum yield was calculated. The results of absorption and emission spectra are presented.

BP 17.19 Tue 18:00 P4

Real-time monitoring of fluctuations in ATP levels and mechanobiological signatures in living cells — •Albina Nizamieva and Matthias Weiss — Experimental Physics I, University of Bayreuth, Bayreuth, Germany

Living cells are genuine non-equilibrium systems with a typical energy turnover of roughly 10^8 times thermal energy in every second. This translates to about 10^7 ATP hydrolysis events per second, with which cells may fuel, for example, signaling cascades and/or contractions of the actomyosin cytoskeleton to probe and migrate on the substrate underneath. Here we have used fluorescent reporter molecules to quantify in living cells (1) the temporally fluctuating ATP levels, and (2) fluctuations of a key mechanosensory protein that connects cellular mechanics and signaling cascades. Our data reveal marked fluctuations on the scale of minutes and beyond, whereas short-term fluctuations appear to only report on fundamental and ubiquitous physico-chemical fluctuations that are rooted, for example, in the dyes' photophysics and diffusional motion.

BP 17.20 Tue 18:00 P4

Microscopic observation of red blood cell band patterns formed by centrifugation — •Luca Hastenteufel, Thomas John, Felix Maurer, and Christian Wagner — Experimental Physics, Saarland University

Percoll is a common medium composed of coated silica particles. It is widely used as the standard medium for the density separation of cells or subcellular compounds. The centrifugation of red blood cells in Percoll exhibits a heterogeneous structure characterized by discrete bands, however the density gradient is continuous. These band patterns have primarily been analysed using macroscopic images, such as photographs. We developed a microscopic scanning setup to examine

these patterns in detail, from single cell level in μm-range up to the full pattern structure at 6 cm. This provides higher-resolution insights compared to traditional imaging methods. Additionally, high dynamic range (HDR) methods using multiple exposure levels lead to a more detailed pattern observation. Understanding these band patterns offers valuable information about red blood cell aggregation energy and the severity of related diseases.

BP 17.21 Tue 18:00 P4

Accessing local aggregation in phalloidin-stained Actin filaments using 2D Polarization Fluorescence Imaging — •Shangjun Cheng[1,2,3], Yutong Wang[1,2], Yunhao Mei[1,2], Hossein Zarei Oshtolagh[1,2], Lukas Spantzel[1,3], Patrick Then[1,4], Hans-Dieter Arndt[1], Adrian T. Press[1,3], Rainer Heintzmann[1,2], and Daniela Täuber[1,2] — [1]Friedrich Schiller University Jena — [2]Leibniz Institute of Photonic Technology, Jena — [3]Jena University Hospital — [4]Microverse Imaging Center, Jena, Germany

2-dimensional polarization-resolved fluorescence imaging (2DPOLIM) can discriminate between aggregated and non-aggregated protein forms independent of the sample's alignment by providing access to the full in-plane polarization properties of the sample. In combination with a semi-quantitative analysis of Förster Resonance Energy Transfer between similar fluorophores (homo-FRET) it can map the local aggregation in cells and tissue [1]. Actin assembly and disassembly is essential for cellular dynamics. A previous study has shown the direct link between infection and aggregation of F-Actin in hepatocytes [2]. Here, we present our speeded-up home-built 2DPOLIM setup [3] along with its calibration and image registration protocols allowing for an acquisition time in the range of a second. First results from application to the investigation of phalloidin-stained Actin filaments are presented. – [1] R. Camacho, et al., Advanced Materials, 31, 1805671, 2019. [2] P. Martinac, et al., Infection, 47, S6-S7, 2019. [3] Y. Wang, et al., Klosters, Switzerland, January 2023. doi:10.13140/RG.2.2.35169.79204

BP 17.22 Tue 18:00 P4

Liquid-cell Scanning Transmission Electron Microscopy (STEM) of isolated mitochondria and respective Au labels — •Eric Lieberwirth[1], Kevin Oldenburg[2], Anja Schaeper[3], Marcus Frank[4], Ingo Barke[1], Simone Baltrusch[3], and Sylvia Speller[1] — [1]Institute of Physics & LLM, University of Rostock — [2]ELMI-MV, University of Rostock — [3]Institute of Medical Biochemistry and Molecular Biology, Rostock University Medical Center — [4]Electron Microscopy Center, Rostock University Medical Center

In situ liquid-cell Scanning Transmission Electron Microscopy (STEM) holds the promise to observe biological organisms in a native state such as organelles, bacteria and eukaryotic cells [1,2]. In addition to acquisition of individual images, movies can be recorded during manipulation of tissue [3]. The potential radiation damage due to the transit of the electron beam through the sample is still under debate [4]. We imaged isolated mitochondria in Krebs-Ringer medium, and extracted imaging performance, and external features of radiation damage. We also study Au labels in the physiologic medium and show that atomic resolution of the nanoparticles is attainable. Such labelling is expected to increase resolution [1] and validate the presence of mitochondria in the STEM. One of the next challenges is validating the metabolic activity of the mitochondria during or upon the (S)TEM measurement.

[1] Kun He et al. (2019) J. Phys.: Condens. Matter 31 103001
[2] Frances M. Ross (2024) Micro. Tod. 32 17-22
[3] Elliot S. Pohlmann et al. (2015) Nano Lett. 15 2329-2335
[4] Yulian Wu et al. (2019) New J. Chem. 43 12548

BP 17.23 Tue 18:00 P4

Three-Axis Structured Illumination Lightsheet Microscopy — •Meelad Lalenejad and Alexander Rohrbach — University of Freiburg, Freiburg, Germany

Light-sheet microscopy (LSM) is known for increased image contrast and reduced photo-bleaching and toxicity since only those parts of the object are illuminated from the side that is in the focus of the objective lens. In addition, larger volumes are scanned plane-wise or line-wise by optimized laser beams, so LSM is significantly faster than point-wise scanning methods. However, for imaging a small number of cells, the spatial resolution is limited by the numerical aperture of the objective lens. We tackle the problem of limited resolution by combining holographically shaped illumination beams with three-axis interferometric arrangements. We use structured illumination microscopy (SIM) to obtain 3D super-resolved images in scattering media by generating interference fringes between every two beams from different illumination objective lenses.

BP 17.24 Tue 18:00 P4

Investigating Neutrophil dynamics using 200 Hz Rotating Coherent Scattering Microscopy — •Vera Obloh and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, Department of Microsystems Engineering (IMTEK), University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

Neutrophils, the largest population of leukocytes in the human bloodstream, are initial responders in the rapid innate immune defense against most bacterial and fungal pathogens. They are activated before the complex humoral and lymphocyte-mediated processes of acquired immunity can effectively respond to an infection. To ensure effective defense, Neutrophils rapidly and efficiently move to areas of infection, based on highly dynamic processes of cytoskeleton reorganisation. Due to their ability to migrate rapidly and their availability and ease of cultivation, HL-60 Neutrophils are well suited for observations with Rotating Coherent Scattering (ROCS) microscopy, a novel 200 Hz label-free imaging technique with resolutions well below 200 nm. ROCS represents a powerful, high-speed alternative to fluorescence microscopy, especially for observations over thousands of frames. We represent first images and analyses of so far unseen details and dynamics of Neutrophil migration.

BP 17.25 Tue 18:00 P4

Characterisation of fluorescent dyes and their uptake by M2 cells using FLIM — •Jana Sütterlin[1], Francisco Páez-Larios[1,2], Lukas Harder[1], Lea Klepsch[3,4], Vivien Bachmann[5], Antje Vollrath[3,4], Paul Jordan[5], Ulrich Schubert[3,4], Oliver Werz[5], Christian Franke[1], and Christian Eggeling[1,2] — [1]Institute for Applied Optics and Biophoysics, Friedrich-Schiller-Universität Jena, Jena, Deutschland — [2]Department of Biophysical Imaging, Leibniz-Institut für photonische Technologien e.V., Jena, Deutschland — [3]Jena Center for Soft Matter, Friedrich-Schiller-Universität Jena, Jena, Deutschland — [4]Institute for Organic and Macromolecular Chemistry, Friedrich-Schiller-Universität Jena, Jena, Deutschland — [5]Department of Pharmaceutical and Medical Chemistry, Friedrich-Schiller-Universität Jena, Jena, Deutschland

Polymeric nanocarriers are used to incorporate active substances into cells, that otherwise would have limited bioavailability. To study the particle-cell-interaction, the nano-particles contain a fluorescent dye, which allows monitoring by fluorescence microscopy. Since a dye's fluorescence lifetime depends on its environment, the dye's release from the nanoparticle into the cellular cytosol can be evaluated temporally and spatially by fluorescence-lifetime-imaging (FLIM). To that end, lifetime behaviour of Nile Red, ATTO 665 and ATTO Rhodamine 3B is characterised under different solvent conditions mimicking different cellular compartments. By this, a comparison with FLIM data of live cell uptakes is possible, which can yield insights into the dynamic interaction of drug-loaded nanoparticles and their target cell.

BP 17.26 Tue 18:00 P4

MINFLUX-derived particle traces reveal Mean Back Relaxation to study active systems — •Deisel Tobias, Muenker Till, Vos Bart, and Betz Timo — Third Institute of Physics, Georg-August Universität Göttingen, Göttingen, Germany

Living systems like cells exhibit dynamics far from thermodynamic equilibrium. In order to study such non-equilibrium systems, we need to use analytical methods beyond the classical methods developed in statistical physics. In order to quantify the activity in a living, we have recently introduced the Mean Back Relaxation (MBR), which exploits a three-point probability function and is solely derived from passive measurements. A main hurdle in using the MBR in the requirement of particle trajectories with high temporal and spatial precision, that are sufficiently long to detect activity. In normal flourescence microscopy this is not possible to achieve because of probe bleaching. To overcome this, we measure the MBR using MINFLUX nanoscopy, which is able to track fluorescent particles at a spatio-temporal resolution in the order of nanometers at a frequency in the order of a few kHz. We explore the MBR of fluorescent particles in living cells and study its change under the influence of cytoskeletal inhibition.

BP 17.27 Tue 18:00 P4

Thermal and directional motion of trapped particles in periodic potentials — •Ellen Hermle and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, Department of Microsystems Engi-

neering (IMTEK), University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

Molecular fiction can be considered as continuous on-binding and off-binding of molecules between two sliding surfaces. This complex process of energy dissipation to the environment, is important on most length scales, time scales and across disciplines. Usually, the relation between dynamic friction and velocity is quantified by a coefficient, which depends on various on- and off-binding parameters. Here, optical tweezers based Photonic Force Microscopy (PFM) has proven to be a suitable technique is used to analyse friction processes on mesoscopic length scales, specially at soft (-bio) interfaces. By 3D interferometric position tracking at 1 MHz we determine mean particle displacements and forces, as well as fluctuations of displacements and forces. Besides Brownian dynamic simulations, we present first experimental results of fluctuating particles dragged through a periodic potential, which can be generated by an optical potential from two interfering beams or by a specifically coated glass surface.

BP 17.28 Tue 18:00 P4

Investigating Ultrasonic Effects on Oral Cancer Cells Using Fluorescence Microscopy — •Wafa Tounsi, Amar Avdakovic, Vivian Maria Gulczynski, and Mathias Getzlaff — Institute of Applied Physics, University of Duesseldorf

Head and neck squamous cell carcinoma (HNSCC) is a challenging and often resilient cancer that affects many people globally. As conventional treatments sometimes fall short of effectively targeting these cancer cells without causing damage to surrounding healthy tissue, our research focuses on finding innovative alternatives. Our contribution explores the potential of using ultrasonic frequencies to selectively affect cancer cells while sparing healthy ones, offering a possible new avenue for treatment. In this study, we investigate how HNSCC cells respond to ultrasonic waves at frequencies between 20 and 250 kHz. We compare their reactions to benign oral keratinocytes, aiming to pinpoint acoustic conditions that might selectively disrupt cancer cells. In combination with Fluorescence Microscopy, we track various cellular responses, including changes in cell shape, membrane stability, and mitochondrial activity, using specific fluorochromes such as CellMask Green for plasma membranes, Hoechst for nuclear staining, and MitoTracker for mitochondria. By observing these differences, especially in the cytoskeleton, we gain valuable insights into the unique vulnerabilities of HNSCC cells, potentially paving the way for ultrasound-based, non-invasive treatments. Exploiting the distinct mechanical properties of cancer cells could enhance patient outcomes by enabling safer, more targeted treatments.

BP 17.29 Tue 18:00 P4

A flavin-based photoreceptor controls the photoactivation of ciliary adhesion in *Chlamydomonas*. — •Rodrigo E. Catalan[1,2], Antoine Girot[1,2], Alexandros Fragkopoulos[1,2], Olga Baidukova[3], Peter Hegemann[3], and Oliver Bäumchen[1,2] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [3]Humboldt University of Berlin, Institute of Biology, 10115 Berlin, Germany.

Light-activated proteins or photoreceptors play a crucial role on the behavior and, ultimately, the survival of photoactive microorganisms. The unicellular biciliated microalga *Chlamydomonas reinhardtii* has become a model organism to study light-mediated phenotypes, such as photosynthesis and phototaxis, among many others. Recently, we discovered that *C. reinhardtii* can reversibly switch on and off the adhesiveness of their cilia in blue and red light, respectively [1,2]. We characterized the action spectrum of this phenotype in wild-type (WT) *C. reinhardtii* cells via single-cell micropipette force measurements, and showed that it resembles the spectral sensitivity of a flavin-based photoreceptor. Further comparison of the ciliary adhesion forces between WT and photoreceptor-targeted mutants reveals that the deletion of two flavin-containing photoreceptors, namely animal- and plant cryptochromes, completely disrupts light-switchable adhesion.

[1] C. T. Kreis *et al.*, *Nat. Phys.* **14**, 45-49 (2018).
[2] R. E. Catalan *et al.*, *Soft Matter* **19**, 306-314 (2023).

BP 17.30 Tue 18:00 P4

Ciliary Adhesion of *Chlamydomonas reinhardtii* on Charge-Functionalized Surfaces — •Lea Rupprecht[1], Rodrigo Catalan[1], Christina Heinritz[2], Thomas Scheibel[2], and Oliver Bäumchen[1] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]University of Bayreuth, Biomaterials, 95447 Bayreuth, Germany

Elucidating the physical phenomena underlying the interactions between microorganisms and surfaces is crucial for developing technologies to control the formation of microbial biofilms. While most studies use bacteria as model organisms, the principles of microbial adhesion remain rather elusive for eukaryotic photosynthetic microorganisms. Recently it was discovered that the model unicellular microalga *Chlamydomonas reinhardtii* adheres to surfaces by means of its two cilia under blue light [Kreis *et al.*, Nature Physics, 2018]. With *in vivo* single-cell micropipette force spectroscopy, the ciliary adhesion forces of *C. reinhardtii* on functionalized substrates were characterized to dissect the influence of surface energy, van der Waals and electrostatic interactions [Kreis *et al.*, Soft Matter, 2019]. The results suggest that the predominant nature of the protein-mediated cilia-substrate adhesion of *C. reinhardtii* is due to electrostatic interactions. Here we present adhesion force measurements of *C. reinhardtii* on poly-L-lysine- and recombinant spider silk-coated silicon, revealing no charge preference for ciliary adhesion. In contrast to prokaryotic microorganisms, our results show *C. reinhardtii* uses highly versatile cilia to achieve microbial adhesion to surfaces of a broad range of physicochemical properties.

BP 17.31 Tue 18:00 P4

Intracellular mechanics in migrating cells — •Jannis Fischer, Mohammad Amin Eskandari, and Timo Betz — Third Institute of Physics, Göttingen, Germany

To fulfill their incredibly large number of different tasks, biological cells have developed mechanisms to adapt their physical properties and appearance. The proper control of these changes is crucial, as they are not only essential for healthy cells, but can also distinguish healthy from diseased cells. Important examples related to such changes in mechanical properties are cell shape variation or cell migration. It is still not clear whether the changes in these mechanical properties are due to passive or active processes. Investigating and understanding these processes is the core of this work. For this, I will analyze the behavior of migrating cells, which are induced to move alternately on patterns and within channels. To connect the observed dynamics with the underlying mechanical properties and activities I will use the new quantity of mean back relaxation (MBR). Findings in this area could provide information for the big question of whether the mechanical properties of cells can be predicted by their activity.

BP 17.32 Tue 18:00 P4

Same, but different: Shared viscoelastic signature in hydrogels and cells — •Dorian Marx, Till M. Münker, Bart E. Vos, and Timo Betz — Third Institute of Physics - Biophysics, Georg-August-Universität Göttingen, Germany

We report the discovery of a striking "mechanical fixed point" in the response of polyacrylamide-based hydrogels to shear strain. Characterized by a pronounced and invariant relationship of parameters of the mechanical model, this leads to a convergence of the complex shear moduli of all measurements at a frequency of approximately 5 kHz. Intriguingly, reviewing existing literature reveals that this phenomenon is not unique to our simple hydrogel. Rather, there are many qualitatively similar observations in the distinct realm of (intra-)cellular mechanics, as probed by diverse techniques including optical tweezers and atomic force microscopy using many different cell types. Despite the fundamentally different natures of these systems - one being passive and at equilibrium (hydrogel), the other active and out-of-equilibrium (cell) - they show this peculiar viscoelastic signature. The existence of the mechanical fixed point hints at an unresolved constraint governing the mechanics across vastly different biological and synthetic systems.

BP 17.33 Tue 18:00 P4

: Identifying the proteins controlling the intracellular active mechanics — •Noémie Veyret, Till Münker, and Timo Betz — Third institute of Physics, University of Göttingen, Germany

Over the past few years, the study of cell mechanical properties has allowed new insights on the understanding of biological processes and life complexity. According to previous work, intracellular mechanical properties can be narrowed down to a fingerprinting of only 6 parameters. Through the use of active and passive microrheology measurements via optical tweezers, frequency dependent viscoelastic properties and intracellular activity were found to vary for different cell types. The aim of this project is to find a correlation between changes in protein expressions and mechanical fingerprint of cells. To do so optical tweezers measurements will be performed during the differentiation process

of induced Pluripotent Stem Cells (iPSCs) into cell types derived from the three germ layers, namely neurons (ectoderm), skeletal muscles (mesoderm) and hepatocytes (endoderm). This measurement allows the characterization of the mechanics during the iPSC differentiation process. In parallel, the cell proteome will be studied using mass spectroscopy. Combining both, we hope to find the connection between proteins and their mechanical role, the intracellular "mechanome".

BP 17.34 Tue 18:00 P4

Investigating the rheology of intracellular transport by magnetic tweezers — •Katharina Beitzinger, Simon Wieland, and Holger Kress — Biological Physics, University of Bayreuth, Germany

Intracellular transport is an important part of phagocytosis, the cellular internalization of extracellular objects such as bacteria or microplastic particles. After uptake, the phagosome is transported mainly by dyneins along microtubules to the perinuclear region as part of the phagosomal maturation process. However, the kinetics of the recruitment of the motors to the phagosome is largely unknown. In order to investigate the mechanics of the transport, we use magnetic tweezers in combination with paramagnetic particles, internalized by mouse macrophages. By switching the tweezers on and off periodically, we exert alternating forces on the particle during the transport. The changes in the local viscoelastic cell properties are determined by modeling the creep compliance with a power law. First experiments show that the viscosity of the cells around the phagosomes remains almost constant, while the stiffness increases over time. The change in stiffness can be an indicator for a progressive adaption of the cell towards external stress by a recruitment of molecular motors to the phagosome. We expect that a quantification of the local viscoelastic cell properties during phagosomal transport can lead to a better understanding of this fundamental cellular process.

BP 17.35 Tue 18:00 P4

Optimizing Microfluidic Synthesis of Polymer Beads for In-Vivo Force Cell Sensing — •Jordan Dieter Groh, Alejandro Jurado Jiménez, and Timo Betz — Drittes Physikalisches Institut, Göttingen, Deutschland

Since the first use of deformable beads inside living tissue as force sensors about ten years ago, the technique has been refined with the introduction of new materials and methods to measure deformation. In many experiments, polyacrylamide beads have been used to assess forces in all kinds of in-vivo and in-vitro systems such as developing embryos, cancer spheroids, or reconstituted muscle tissue. However, using shear-induced emulsions as a fabrication method still shows two main limitations: a broad size distribution and small variations in polymer stiffness. We were able to optimize the production of polyacrylamide beads in two ways. First, by adoption of flow-focusing in a microfluidic setup. This technique is commonly employed in diverse fields, including drug delivery and food industry, for creating emulsions with precise control over droplet sizes. Second, by the use of a UV light-sensitive polymerization initiator that was triggered after the emulsion was created. The UV initiation of polymerization is instrumental in avoiding clogging of the microfluidic chips as polymerization happens only after emulsification. These improvements resulted in large beads with diameters of 93 um, which are still too large for many applications. Current approaches aim to reduce the bead size to around 5 um or even below.

BP 17.36 Tue 18:00 P4

Characterizing diffusion properties at liquid-liquid interfaces in microfluidic channels — •Eric Schneider, Eric Sündermann, Bob Fregin, and Oliver Otto — Institute of Physics, University of Greifswald, Greifswald, Germany

Real-time deformability cytometry is a powerful and widely used method for investigating the mechanical properties of cells in suspension. Here, cells are deformed by hydrodynamic stress in a microfluidic system, that is comparable in size to the cells. Consequently, the range of cell sizes has to match the physical channel dimensions to ensure proper cell deformation. Virtual fluidic channels (VFCs) address this limitation, by allowing for the channel width to be adjusted within seconds. VFCs are formed by the liquid-liquid interface between two co-moving aqueous polymer solutions. The introduction of these two different polymer solutions generates a density gradient within the microfluidic channel, which can give rise to diffusive processes. We investigated the diffusive properties within VFCs and the influence of the liquid-liquid interface. For this, we examined the temporal behavior of a fluorescent dye distribution within the microfluidic chip. We modelled the diffusive behavior self-consistently by solving the kinetic diffusion equation, which accounts for the differential flow velocities within the microfluidic channel. Finally, by combining theoretical and experimental results, we determine the characteristic diffusion timescales in the VFC and across the liquid-liquid interface. With this we provide a general framework to investigate the diffusive properties along laminar flow boundaries.

BP 17.37 Tue 18:00 P4

A fast and quantitative method to study the membrane tension of suspended cells — •Eric Sündermann, Bob Fregin, Doreen Biedenweg, and Oliver Otto — Institute of Physics, University of Greifswald, Greifswald, Germany

The development of high-throughput methods for cell mechanical research is becoming increasingly important as the analysis of large samples improves the statistical robustness to identify rare cell populations and transfer results from basic science into clinical applications. Various techniques are available for bulk mechanics, but none can analyse membrane tension with the throughput of a flow cytometer.
Here, we present membrane tension cytometry (MTC), that uses Flipper-TR, a fluorescent dye with a fluorescence lifetime being proportional to the tension inside a lipid bilayer. First, we established a calibration procedure using osmotically-stressed red blood cells. Next, we move to HL60 cells, a myeloid precursor cell line, which we exposed to various chemical and mechanical stresses. We find an increased fluorescence lifetime for increasing hydrodynamic stresses, as expected. Finally, we used methyl-β-cyclodextrin and Cytochalasin D to disturb cholesterol and filamentous actin levels, respectively. Our results show, that MTC is sensitive to membrane changes while being insensitive to cytoskeletal alterations.

BP 17.38 Tue 18:00 P4

Thermomechanical properties of bat erythrocytes as a blueprint for human hibernation — •Bob Fregin[1,2], Doreen Biedenweg[1], Oliver Otto[1,2], and Gerald Kerth[3] — [1]Institute of Physics, University of Greifswald, Greifswald, Germany — [2]German Center for Cardiovascular Research, Partner Site Greifswald, Greifswald, Germany — [3]Applied Zoology and Nature Conservation, Zoological Institute and Museum, University of Greifswald, Greifswald, Germany

The ability to sustain efficient blood circulation at low body temperatures is a critical adaptation in hibernating mammals. Here, the mechanical properties of red blood cells (RBCs) could play a crucial role, which we studied for the hibernating common noctule bat, the non-hibernating Egyptian fruit bat, and humans. Using dynamic real-time deformability cytometry RBC elasticity and viscosity were measured at physiologically-relevant time scales (Milliseconds) and temperatures (37°C, 23°C, and 10°C).

Our findings reveal a temperature-driven increase in elasticity and viscosity, which is mainly influenced by membrane properties and not the cytosol. This effect is significantly enhanced in bats. Finally, our data demonstrate that RBC membranes of both bat species display a transition to a viscous-like state at lower temperatures, which is not explained by seasonal variations of environmental factors but seems to originate from physical properties of the cell membrane. Our results suggest RBC thermomechanical properties as a target for future research on human hibernation.

BP 17.39 Tue 18:00 P4

Passively Measuring Cell Activity via Mean Back Relaxation — •Sarah Louisa Lädke[1], Till Moritz Münker[1], Julian Schulz[1], Gabriel Knotz[2], Matthias Krüger[2], and Timo Betz[1] — [1]Third Institute of Physics, Georg-August-Universität Göttingen — [2]Institute of Theoretical Physics, Georg-August-Universität Göttingen

While many statistical methods are available for the characterization of passive motion in thermodynamic equilibrium, the investigation of active motion in living systems remains a significant challenge. In particular, the study of intracellular mechanical properties requires techniques such as active microrheology to quantify the response of tracer particles to forces exerted via optical or magnetic tweezers. However, these methods often involve expensive and complex equipment, and their invasive nature can alter cellular behavior.

To address these limitations, we present an alternative approach to study intracellular mechanical properties and activity that relies only on passive measurements. To this end, we combine darkfield microscopy, highspeed imaging and image post-processing techniques to

obtain trajectories of microparticles in Hela cells with nanometer and 300 microseconds spatial and temporal resolution. To filter noise that occurs in our particle tracking, we developed a new, Bayesian approach that can reliably differentiate between noise peaks and intrinsic fluctuations found in the frequency spectrum. Using the novel observable Mean Back Relaxation (MBR), we can link the particle tracks to intracellular activity and their mechanical properties.

BP 17.40 Tue 18:00 P4

Competition between deformation and free volume quantified by 3D image analysis of red blood cell — •Pavlik Lettinga[1,2], Mehrnaz Babaki[1,2], Dmitry Fedosov[1], Amirezza Gholivand[1], Remco Tuinier[3], and Joeri Opdam[3] — [1]Forschungszentrum Jülich — [2]KU Leuven — [3]TU Eindhoven

Cells in living organisms are subjected to mechanical strains caused by external forces like overcrowding, resulting in strong deformations that affect cell function. We study the interplay between deformation and crowding of red blood cells (RBCs) in dispersions of nonabsorbing rod-like viruses. We identify a sequence of configurational transitions of RBC doublets, including configurations that can only be induced by long-ranged attraction: highly fluctuating T-shaped and face-to-face configurations at low, and doublets approaching a complete spherical configuration at high, rod concentrations. Complementary simulations are used to explore different energy contributions to deformation as well as the stability of RBC doublet configurations. Our advanced analysis of 3D reconstructed confocal images of RBC doublets quantifies the depletion interaction and the resulting deformation energy. Thus, we introduce a noninvasive, high-throughput platform that is generally applicable to investigate the mechanical response of biological cells to external forces and characterize their mechanical properties.

BP 17.41 Tue 18:00 P4

Red blood cell membrane tension modulation by photo switchable molecules — •Tim Kutz[1], Bart Vos[1], Jan Bart Ravoo[3], Andreas Janshoff[2], and Timo Betz[1] — [1]Third Institute of Physics, Georg August Universität Göttingen, Göttingen, Germany — [2]Institute of Physical Chemistry, Georg August Universität Göttingen, Göttingen, Germany — [3]Organic Chemistry Institute and Center for Soft Nanoscience, University of Münster

Cellular stiffness and surface tension are fundamental determinants of cell behavior and function. However, the precise contributions of membrane and cortical components to overall cell mechanics remain unclear. Building upon our recently developed multi-modal approach, which combines atomic force microscopy, confocal spinning disk fluorescence microscopy, and micropipette aspiration, we investigated the mechanical properties of human red blood cells (hRBC) as a model system, with a focus on membrane manipulation. By incorporating photo switchable azobenzenes into the hRBC membrane, we created a dynamic system to modulate membrane properties through light-induced conformational changes.Comparisons were made between wild-type hRBCs and those containing azobenzenes in both the cis and trans states. This approach enabled us to directly correlate changes in membrane conformation with alterations in mechanical properties. Our results demonstrate the feasibility of using photo switchable molecules to modulate cellular mechanics in a controlled and reversible manner. This approach and novel platform advances our understanding of the contribution of the membrane to cellular tension.

BP 17.42 Tue 18:00 P4

Theoretical perspectives on controlling cells by ultrasound — •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, 69120 Heidelberg, Germany

Aside from the well-known use of ultrasound in medical imaging, there are many other biomedical applications of ultrasound, including enhanced bone healing, neurostimulation and sonogenetics. Different mechanisms have been implicated for these processes, including temperature changes, cavitation, radiation forces and acoustical streaming. In this work, we are interested in the interaction between ultrasound and tissue (including organoids) at the single-cell level. Combining concepts from hydrodynamics, elasticity theory and soft matter, we aim at theoretical predictions of the relative relevance of these different effects. In particular, we use the theory of viscoelasticity to predict whether intracellular streaming and organelle movement can be controlled by ultrasound.

BP 17.43 Tue 18:00 P4

Predicting mass density of eukaryotic nuclei and cells — •Omar Muñoz[1,2,3], Abin Biswas[1,3,4], Kyoohyun Kim[1,3], Jochen Guck[1,3], Vasily Zaburdaev[1,2], and Simone Reber[4,5] — [1]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany. — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [3]Max Planck Institute for the Science of Light, Erlangen, Germany — [4]Max Planck Institute for Infection Biology, Berlin, Germany — [5]University of Applied Sciences Berlin, Berlin, Germany

Biophysical properties of the cell nucleus are important for various cellular processes from transcription to migration, but largely are still not well understood. The mass density is one such example, since we observed for a wide range of species that the cells maintain a certain nuclear to cytoplasmic mass density ratio with nuclear mass density being lower than its cytoplasmic counterpart. Moreover, in diseased states such as senescence we observed a breakdown of this density ratio where dilution of the cytoplasm made nuclei appear more dense, which suggests that the density ratio is a potential marker of proper cell functionality. Theoretical modeling can contribute to a better understanding of how this density ratio is established. There are two essential model components: a pump leak model to predict compartment volume and a model to determine the dry mass in the system, which is usually an active, dynamic process. Here we present the models for different systems such as human cells, nuclei in Xenopus egg extract and discuss their differences.

BP 17.44 Tue 18:00 P4

Modeling the endothelial cytoskeleton response to blood flow — •Berin Becic and Stephan Gekle — Biofluid Simulation and Modeling, University Bayreuth, Germany

As present in blood flow, it was observed that a shear flow leads to an alignment of endoethelial cells, which is connected to an alignment of its cytoskeleton. Understanding this behavior is important as its failure can lead to chronic inflammation which is one cause for the formation of artherosclerosis and other cardiovascular diseases. In order to do this we develop a three-dimensional model for the formation of the cytoskeleton based on the stress- and strain-dependency of the stress-fiber association and dissociation dynamics, as proposed by Deshpande et al (A bio-chemo-mechanical model for cell contractility , PNAS 2006). This model also offers the opportunity to study the spatially resolved formation of the cytoskeleton as observed in cells adhering to a substrate or the mechanic interactions between the cell and its nucleus.

BP 17.45 Tue 18:00 P4

Combining computational and experimental advances in microparticle traction force microscopy — •Bastian Kraus[1], Simon Brauburger[1], Tobias Walther[2], Kerstin Göpfrich[2], and Ulrich S. Schwarz[1] — [1]Institute for Theoretical Physics, Heidelberg University, 69120 Heidelberg, Germany — [2]Center for Molecular Biology of Heidelberg University (ZMBH), Heidelberg University, 69120 Heidelberg, Germany

Traction force microscopy (TFM) infers cellular forces from the motion of fiducial markers embedded in soft elastic substrates. Over the last years, this approach has been extended to elastic microparticles, typically made from polyacrylamide. In contrast to flat substrates, this approach allows to infer forces either from the motion of embedded fiducial markers or from the deformation of the surface. Here, we compare these two different approaches from the viewpoint of elasticity theory and with computer simulations that include the image processing steps. We then apply the method to experimental data from DNA microbeads, for which one can implement markers for both bulk and surface deformations.

BP 17.46 Tue 18:00 P4

An FEM based framework to reconstruct cellular traction forces in arbitrary geometries — •Cornelis Mense and Ulrich Schwarz — Heidelberg University

In the last two decades, the reconstruction of cellular traction forces has been a valuable tool in mechanobiology and biomedical experiments. Traction forces are traditionally computed for displacements of soft elastic substrates, imaged using fluorescent micro-beads. These substrates have largely been planar surfaces, owing to the availability of methods by which to analyse such experimental data. But, as of late,

a curiosity and drive has arisen to extend these experiments to arbitrary three-dimensional geometries. Here, a framework is proposed to inversely reconstruct tractions using the Finite Element Method. This method attempts to reduce noise and non-physical tractions by iteratively projecting experimental displacement fields onto force-balanced configurations using the principle of virtual work. The efficacy of the method is demonstrated through toy problems, wherein tractions are first prescribed onto a geometry to generate mock data sets of displacement fields. These fields are then artificially made noisy, after which the FEM software is tasked with retrieving the initially prescribed tractions. The experimental design space, that would be opened up by this framework, could prove a valuable tool in further understanding cell motility.

BP 17.47 Tue 18:00 P4

Investigating Particle Binding above Epithelial Cells with Photonic Force Microscopy — Nils le Coutre and •Alexander Rohrbach — IMTEK, Department for Microsystems Engineering, Freiburg, Germany

A significant portion of today's airborne particulates originates from human activities such as industrial processes and the combustion of crude oil-based fuels. This has been linked to an increased risk of diseases including asthma, lung cancer, and cardiovascular pathologies, correlating significantly with the inhalation of particulate matter. Here, we investigate the fluctuation-based interaction of single optically trapped particles with epithelial cells. Using photonic force microscopy, we trap the particles through a layer of epithelial cells and interferometrically track the thermal motions of the particle with the goal to recover binding and friction parameters in contact with the cell surface. This approach is challenging since the cell perturbs the phase of the trapping and tracking beam, such that the characteristic trajectories - obtained by interference and encoding the interactions - require a novel analysis method.

BP 17.48 Tue 18:00 P4

Investigating cell membrane tension — •Tina Boric[1,2], Julia Butzke[1,2], Eva Kreysing[2,3], and Kristian Franze[1,2,3] — [1]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [2]Institute of Medical Physics and Microtissue Engineering, Friedrich-Alexander-Universität, Erlangen-Nürnberg, Erlangen, Germany — [3]Department of Physiology, Development and Neuroscience, University of Cambridge, Cambridge, UK

Cellular membranes are known to change their mechanical properties in response to external and internal mechanical stimuli, such as shear forces and changes in tissue stiffness. Membrane tension contributes to the transduction of these mechanical signals into intracellular responses via mechanosensitive ion channels. However, how and if a change in tissue stiffness affects the surface mechanics of the cell, which in turn would contribute to the activation of mechanosensitive ion channels, is not yet known. We are investigating the dependence of the effective membrane tension of HEK 293T cells on the expression levels of the mechanosensor Piezo1 using optical tweezers. Furthermore, we are comparing tether forces of cells grown on compliant custom-made substrates of biologically relevant stiffness. We also expose the cells to different pharmacological treatments that primarily affect the actin cortex to investigate how membrane-to-cortex attachment affects tether forces. Ultimately, our aim is to understand how changes in membrane tension lead to the activation of Piezo1. Our work will contribute to the understanding of how mechanosensitive ion channels are gated, which may have important implications for drug design in the future.

BP 17.49 Tue 18:00 P4

Revealing minimal cell particle interactions by thermal noise frequency decomposition — •Max Wechlin, Felix Jünger, and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, Department of Microsystems Engineering (IMTEK), University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

Nearly every interaction process in nano-scale soft materials, especially in living cells is governed by thermal noise. However, it is hardly known or often disregarded that many interaction processes take place only on specific timescales. This means that observing or measuring on the wrong timescale, can lead to wrong results or even no results. While interactions can be visible on one timescale, they can be completely invisible on another. Therefore, it is not only necessary to measure on a much broader frequency range than usually, but also to decompose the broadband fluctuation data with appropriate mathematical models. This way minimal or even hidden interactions can be revealed. We use optical tweezers based Photonic Force Microscopy with MHz-rate interferometric 3D particle tracking to approach 1*m-sized polystyrene beads to functional gels or to living cells. We demonstrate that interactions between particles and cells change in stiffness or friction over time and distance only on certain frequency bands, but not over the average fluctuations in energy and position.

BP 17.50 Tue 18:00 P4

Regulation of plasma membrane tension through the actin cytoskeleton and hydrostatic pressure — •Yogishree Arabinda Panda and Elisabeth Fischer-Friedrich — Excellence Cluster Physics of Life, TU Dresden, Dresden, Germany

The plasma membrane and its associated proteins serve as a critical signaling hub, transmitting information between the extracellular environment and the intracellular space. It plays essential roles in regulating the intracellular ion content, the membrane potential and processes such as endocytosis and exocytosis. Consequently, the plasma membrane is central to many physiological processes including cell differentiation, migration, and proliferation. Recent studies have shown that the activity of many transmembrane proteins is influenced by mechanical tension in the plasma membrane. Despite its importance in cellular signaling, the mechanisms by which cells regulate membrane tension remain poorly understood. In this study, we investigate the regulation of plasma membrane tension in mitotically arrested cells using FLIM in conjunction with the membrane dye FlipTR. Specifically, we explore how components of the actin cytoskeleton, intracellular hydrostatic pressure, and cell shape contribute to both actual and apparent membrane tension.

BP 17.51 Tue 18:00 P4

Single-cell physical phenotyping of blood and tissue biopsies — •Marketa Kubankova[1,2], Despina Soteriou[1,2], Martin Kräter[1,2], and Jochen Guck[1,2] — [1]Max Planck Institute for the Science of Light, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

Deformability cytometry [1] is a microfluidic technique that allows the assessment of physical properties of single cells in a label-free and high-throughput manner, with up to 1000 cells analysed per second. Cell deformation and other physical phenotype parameters such as cell size and aspect ratio are obtained directly from brightfield cell images.

The diagnostic potential of deformability cytometry was previously demonstrated in various diseases [2, 3]. Here we show how deformability cytometry accurately discriminates between healthy and tumorous tissue in biopsies of mouse and human colons [4]. Cell deformation was a crucial parameter for the correct distinction of tumour tissue in colon cancer patients. Furthermore, we present new findings on how the physical properties of blood cells change during infectious diseases, and how they correlate with commonly used markers of infectious inflammation. Our findings pave the way for establishing deformability cytometry as a fast and marker-free diagnostic technique to sensitively detect pathological changes in solid and liquid biopsies.

[1] Otto et al., Nature Methods (2015), [2] Toepfner et al., Elife (2018), [3] Kubánková et al., Biophysical Journal (2021), [4] Soteriou and Kubánková et al., Nature Biomedical Engineering (2023)

BP 17.52 Tue 18:00 P4

Mechanobiology of immune cell confined migration — •Fatemeh Abbasi[1], Timo Betz[2], and Eva Kiermaier[1] — [1]LIMES Institute, University of Bonn, Bonn, Germany — [2]Third Institute of physics, University of Göttingen, Göttingen, Germany

In vivo, cells experience complex tissue environments and have to adjust their behavior and function based on their surrounding. Immune cells are the renowned examples. On their way from the bone marrow, where they are born, to the infection site, they have to cope with various physical challenges including geometrical confinement and different mechanical properties of the host tissues. To perform a successful confined migration, cells need to squeeze their nucleus, the most stiff and largest cell organelle, as well as reorganize their cytoskeleton. Despite the importance of this subject in immunology and pathology, it is still not well-understood how immune cells can adopt different nuclear morphologies and cytoskeleton organization while migrating through the small junctions and pores. Here, we use CFM (Confinement Force Microscopy), which was developed in the lab of Timo Betz, to confine immune cells in a 2.5D environment of various stiffness. We will study the role of centrosome, microtubule and nuclei morphology in innate immune cell confined migration. This study can help us to find out how nuclei and cytoskeletal organelles facilitate immune cell

migration through confined microenvironments of different mechanical properties. Simultaneous measurement of the cell forces on the microenvironment will enable us to find out the mechanobiology of immune cell confined migration.

BP 17.53 Tue 18:00 P4

Processivity of myosin assemblies: ATP dependence and effect on network dynamics — •Jaskaran Singh and Stefan Klumpp — University of Göttingen, Institute for the Dynamics of Complex Systems, Göttingen,Germany

Motors proteins like myosin, kinesin are a major source of activity in cellular mechanisms like cell division and perform tasks such as maintaining cellular structure and transporting cargo within the cell. These motors form complexes of multiple motors and cooperate and give rise to complex behaviors not seen in single-motor dynamics. Myosin motors form medium sized (˜100 motors) assemblies called myosin minifilaments that bind to and move along actin filaments. The mechanochemical cycle of individual motors in the motor assembly is dependent on ATP. We are exploring the concentration of ATP as a control parameter for the processivity (walking distance) of myosin minifilaments through stochastic modelling. Here we propose processivity as a parameter to tune the activity in system. On the cellular scale, we explore the effect of processivity on cytoskeletal network structures at large. Preliminary results show that decrease in ATP concentration increases the processivity of myosin assemblies. However, the velocity of motor assembly decreases with decreasing ATP. Thus, an optimal trade-off between processivity and velocity must be maintained for efficient assembly performance. To study the effect of processivity on network level structures, we use the simulation package Cytosim. The simulation shows that higher processivity leads to a more pronounced contraction of the actin network.

BP 17.54 Tue 18:00 P4

Mechanosensing and shape adaption of cells on substrates of varying stiffness — •Pooja Yadav, Florian Rehfeldt, and Matthias Weiss — Experimentalphysik I,University of Bayreuth

Changes of characteristic cellular features with varying stiffness of the underlying substrate, e.g. shapes and sizes of cells and nuclei, are a hallmark of the complex interplay of mechano-biochemical feedback loops. To explore this in detail, we have quantified cellular features on polyacrylamide (PA) hydrogels of varying stiffness, from 2∼kPa to 64∼kPa, hence mimicking the diverse micro-environments found in vivo. In particular, we have quantified the areas of nuclei and cells, their aspect ratio, and the local order parameter of the cytoskeleton on different substrates, also in the absence and presence of cytoskeleton-severing drugs. As a result, we observed that cell and nucleus areas follow an isometric relation with both areas increasing with the stiffness of the substrate. In contrast, the aspect ratio of both show a non-trivial maximum at intermediate stiffnesses, which we attribute to the local nematic ordering of the cytoskeleton. Altogether, our data open up the way to investigate differential mechanical effects of nuclei and cells under perturbations.

BP 17.55 Tue 18:00 P4

Mechanical properties of microtubule in actin network — •Komal Bhattacharyya, Sarah Köster, and Stefan Klumpp — University of Göttingen, Göttingen, Germany

The cytoskeleton provides structural support and facilitates dynamic cellular processes such as growth and migration. Actin and microtubules are key components of the cytoskeleton. Actin, characterized by its semi-flexible nature, contrasts with the stiff, rod-like structure of microtubules. The synergy between these two elements plays a pivotal role in numerous biological phenomena. For instance, microtubules exhibit enhanced resistance to compressive forces when integrated into an actin network.

In our research, we use the simulation package Cytosim to study composite networks formed by actin and microtubules. Specifically, we analyze the buckling behavior of microtubules under compressive forces and thermal fluctuations and how it is affected by mechanical coupling to actin. We observe that long-range repulsive interactions between the filaments lead to very small elasticity and minimal suppression of microtubule buckling. As a consequence, the observed mechanical responses within composite networks can very likely not be explained without considering specific interactions between actin and microtubules.

BP 17.56 Tue 18:00 P4

Mechanical Properties of Intermediate Filament Networks — •Jonas Penning and Stefan Klumpp — Institute for Dynamics of complex systems, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The mechanical strength and dynamics of cells are essential for sustaining life. For instance, during simple activities such as breathing or walking, cells are subjected to significant tensile stresses as they are stretched, sheared, or compressed. The cytoskeleton - a cross-linked composite network of actin, microtubules, and intermediate filaments - plays a central role in determining the cells' mechanical properties. While actin and microtubule networks have been studied extensively, this work focuses on intermediate filaments, such as vimentin and keratin. Compared to actin, intermediate filaments exhibit much smaller persistence lengths, but are much more stretchable with highly nonlinear elasticity. Extedning the freely-jointed chain (FJC) model by nonlinear stretching elasticity, a simplified model has been developed to investigate the mechanical and physical properties of cross-linked intermediate filament networks. Analogous to experimental approaches, the mechanical properties of the model are tested by applying normal and shear strains or stresses and analyzing the resulting responses.

BP 17.57 Tue 18:00 P4

Infrared Spectroscopic Analysis of Structural and Thermal Dynamics in Cytochrome c-DNA Complex — •Berken Hamarat, Damla Melisa Balci, and Günnur Güler — Biophysics Laboratory, Department of Physics, Izmir Institute of Technology, Izmir, Türkiye

Cytochrome c (Cytc) plays a crucial role in cellular respiration and apoptosis, with potential for biosensor applications due to its electron transfer capabilities. The binding of Cytc to DNA enables its consideration as a target molecule in biosensors and facilitates the modulation of Cytc's electronic properties via protein-DNA interactions. Temperature-controlled FT-IR spectroscopy in the transmission mode was used to investigate the structural changes and thermal stability of Cytc upon DNA complex in oxidized and reduced forms. Deuterated samples of Cytc and DNA were used during the analysis. Structural changes were observed after DNA binding, with a reduction in α-helix content, particularly in the oxidized form. Thermal stability analyses showed that the Cytc-DNA complex lost structural integrity at lower temperatures compared to free Cytc. These results indicate that DNA binding not only alters Cytc's secondary structure but also reduces its thermal stability. While Cytc's high thermal stability makes it suitable for biosensor applications, the observed changes after DNA binding, particularly the decrease in thermal stability must be minimized and optimized to ensure effective biosensor functionality. (Supported by Scientific and Technological Research Council of Türkiye, TÜBITAK 2209-B Project, 1139B412200835).

BP 17.58 Tue 18:00 P4

Soft-landing Electrospray Ion Beam Deposition (ES-IBD) allows integration of native mass spectrometry and cryoEM to investigate membrane protein structure and function — •Carl von Hallerstein, Sophie Lawrence, Tarick El-Baba, Stephan Rauschenbach, and Carol Vivien Robinson — Kavli Institute for Nanoscience Discovery, University of Oxford, UK

Electrospray Ion Beam Deposition (ES-IBD) is an emerging sample preparation for the imaging of molecules (Esser et al. 2022, Faraday Discussions). Recently, using native mass spectrometry (nMS), the deposition and cryo-electron microscopy (cryoEM) imaging of soluble proteins was demonstrated (Esser et al. 2024, Sci. Adv.).

Here, we apply ES-IBD + cryoEM to membrane proteins, which only retain their native state while encased in lipid membranes or membrane-mimetics such as detergents or nanodiscs. ESIBD+cryoEM yields valuable information on lipid and surfactant interaction as well as hydration of the membrane protein.

BP 17.59 Tue 18:00 P4

Investigation into the dynamic structure of heat shock proteins using electrospray ion beam deposition and cryo-electron microscopy (ESIBD+cryoEM) — •Noor Naseeb, Lukas Eriksson, Jingjin Fan, Justin Benesch, and Stephan Rauschenbach — University of Oxford, Oxford, United Kingdom

The heat shock protein (HSP) family encompasses a wide variety of polydisperse proteins that act as chaperones in the cell as a means of preventing aggregation and misfolding of proteins under different forms of cellular stress. Standard methods, like X-ray crystallography

(XRC), Nuclear magnetic resonance (NMR), and cryogenic electron microscopy (cryo-EM), lack the ability to properly study the structures of such dynamic and diverse proteins. To address this, we use electrospray ion beam deposition (ESIBD) that couples native mass spectrometry (MS), a chemically selective sample preparation technique, with cryo-EM. The combination allows for high-resolution visualization of a specific protein assembly by cryo-EM in their near-native state. Here we show that the chemically selective sample preparation technique via ESIBD enables structure determination of these dynamically assembled HSPs can be performed to better assess their structure, and therefore, function.

BP 17.60 Tue 18:00 P4

Hyperfine spectral diffusion in pulse EPR: theory and applications — •Sergei Kuzin[1,2], Gunnar Jeschke[1], and Maxim Yulkov[1] — [1]ETH Zurich, Zurich, Switzerland — [2]MPI for Multidisciplinary Sciences, G\"ottingen, Germany

Hyperfine interaction with nuclear spin bath and nuclear spin-spin interaction often dominate phase memory times of the electron spins in spin-diluted solids at cryogenic temperatures. Such an spin-ensemble effect also manifests is different EPR experiments as spectral diffusion.

Here, we present a new pulse EPR method called intermolecular hyperfine relaxation-induced dipolar modulation enhancement (ih-RIDME). This technique allows to investigate kinetics of spectral diffusion in amorphous solids. The sensitivity range of ih-RIDME lies within 1-3~nm around the spin centre. This makes it a powerful tool to probe nuclear spin arrangement at intermediate electron-nuclear distances. The quantification in ih-RIDME is based on a developed mathematical model of spectral diffusion resulting in a diffusion-like equation. With its help, ih-RIDME allows to quantify heterogeneous systems with a distribution of local proton densities.

We discuss the applications of ih-RIDME in dynamic nuclear polarization, structural biology, spin-labeled macromolecules and soft matter study.

BP 17.61 Tue 18:00 P4

Electron spin dynamics during MW pulses studied by 94 GHz chirp and phase-modulated EPR experiments — •Marvin Lenjer[1,2], Nino Will[3], Fabian Hecker[4], and Marina Bennati[1,2] — [1]MPI for Multidisciplinary Sciences — [2]Georg August University Göttingen — [3]Aarhus University — [4]Danish Technical University

Over the last decade, shaped microwave (MW) pulses have evolved into valuable tools for electron paramagnetic resonance (EPR) spectroscopy. They have been used to improve existing experiments by providing tunable broadband or band-selective frequency profiles as well as to design new experimental approaches. However, most applications were done at low fields (X- or Q-band) where high MW powers are available.

Here, we show the implementation of chirped and phase modulated pulses at a commercial Bruker E680 W-band (94 GHz) EPR spectrometer using a SpinJet arbitrary waveform generator. We apply these novel experimental tools to the analysis of spin dynamics during MW spin lock pulses. We measure inversion profiles in the intermediate regime between Rabi oscillations and saturation pulses via chirp echo EPR spectroscopy and analyze spin-spin relaxation during spin locking (i.e. $T_{2\rho}$) via phase modulation echoes during spin lock. Combination with density matrix simulations allows us to better understand electron spin evolution during long periods of MW irradiation. Altogether, these results promise future advances in design and applicability of hyperfine spectroscopy at high fields by use of spin locks and shaped pulses.

BP 17.62 Tue 18:00 P4

Human cardiac cadherin desmocollin 2 reveals ideal-, slip- and catch bonds in vitro — •Manuel Göz[1], Greta Pohl[2], Sylvia Steinecker[1], Volker Walhorn[1], Hendrik Milting[2], and Dario Anselmetti[1] — [1]Experimental Biophysics & Applied Nanoscience, Faculty of Physics, Bielefeld University, Bielefeld, Germany — [2]Heart & Diabetes Center NRW, University Hospital of the Ruhr-University Bochum, Bad Oeynhausen, Germany

Desmosomal cadherins like DSC2 are known to associate in a strand-swap binding motif in which an N-terminal tryptophan residue binds into the hydrophobic binding pocket of opposing cadherins. Although this binding pattern is highly specific, it is of low affinity and exhibits decreased bond lifetimes at a single-molecule level. Using AFM-based SMFS, we show that the strand-swap dimerized DSC2 has two further binding modes, which may play a role in the integrity of the cardiac muscle. At short interaction times, the DSC2 monomers associate only short-lived and force-independent. These ideal bonds are probably a precursor state that stabilizes the formation of the strand-swap dimer. Tryptophan added to the measurement buffer acts as a competitive inhibitor, preventing the N-terminal strand exchange. Here, DSC2 dimerizes as an X-dimer and shows a triphasic slip-catch-slip type of dissociation. Within a force-activated transition (catch) regime, DSC2 dimers switch between brittle low force and strengthened high force adhesion states. So we can assume that desmosomal adhesion is mediated not only by strand-swap dimers (slip bond) but also by their precursor states (ideal bond) and force-activated X-dimers (catch bond).

BP 17.63 Tue 18:00 P4

Trajectories of particles trapped in double well potentials show new behavior in the Mean Back Relaxation — •Christian Muñoz[1], Mohammad A. Eskandari[1], Bart E. Vos[1], Till M. Münker[1], Dorian Marx[1], Matthias Krüger[2], and Timo Betz[1] — [1]Third Institute of Physics - Biophysics, Georg August University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institute for Theoretical Physics, Georg August University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Optical tweezers have been established as a powerful tool for studying microscopic particle dynamics in complex potentials. In this work, we investigate the behavior of a microparticle trapped in a double-well potential generated by optical tweezers. By systematically varying the laser power and the distance between the optical traps, we modeled the shape and depth of the potential. This approach allowed for a detailed analysis of the particle's stochastic transitions between the wells. Combining experimental measurements with Kramers' theory, we achieved accurate predictions of the transition rates between wells. Furthermore, we analyzed particle trajectories using the new quantity of Mean Back Relaxation (MBR), providing insights into the effects that a bistable system has on particle relaxation after defined fluctuations.

BP 17.64 Tue 18:00 P4

Cell-cell interactions of swimming ciliated microbes: from measured interaction dynamics to an effective potential — •Henrik Groh[1,2], Alexandros A. Fragkopoulos[1], Colin-Marius Koch[3], Michael Wilczek[3], and Oliver Bäumchen[1] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]University of Bayreuth, Experimental Physics I, 95447 Bayreuth, Germany — [3]University of Bayreuth, Theoretical Physics I, 95447 Bayreuth, Germany

In suspensions of living microorganisms the interactions of individual agents may result in large-scale collective effects. Frequently such phenomena are studied more extensively with the goal of linking them to the microscopic single-cell motility and cell-cell interactions. *Chlamydomonas reinhardtii* represents a unicellular eukaryotic model organism that is used to study collective phenomena of puller-type microswimmers, e.g., induced by a self-generated oxygen gradient [1] or by light (phototaxis). In order to complement these studies with a systematic cell-cell interaction analysis, we investigated the mutual interactions of *C. reinhardtii* in a quasi-2D suspension with high temporal and spatial resolution. Our measurements allow for deriving a pair-correlation function and an effective potential, which may eventually enter simulation studies. With our study we provide more detailed insights into the cell-cell interactions of *C. reinhardtii* and thus enable a better understanding of collective phenomena in living suspensions. [1] A.A. Fragkopoulos, et al., *J. R. Soc. Interface* **18**, 20210553 (2021).

BP 17.65 Tue 18:00 P4

Quantum Physics Meets Epigenetics: Does Nature Harness Charge and Energy Transfer in Methylated DNA? — •Dennis Herb[1,2], Mirko Rossini[1,2], and Joachim Ankerhold[1,2] — [1]Institute for Complex Quantum Systems, Ulm University, Germany — [2]Center for Integrated Quantum Science and Technology (IQST), Ulm-Stuttgart, Germany

Charge transfer processes through DNA play a crucial role in gene regulation, including processes such as DNA methylation, an epigenetic modification essential for gene expression. However, the effects of methylation on excitonic energy transfer (EET) and coherent charge transfer (CT) in DNA remain poorly understood. Here, we theoretically investigate the effects of DNA methylation, as well as conformational changes, on biologically relevant DNA sequences. Using a Linear Combination of Atomic Orbitals (LCAO) approach, we compute the molecular electronic structure of nucleic acid bases and derive parameters for a computationally efficient tight-binding (TB) model.

Our model incorporates intrinsic relaxation mechanisms for excited states, mimicking internal conversion (IC), and electron-hole Coulomb interactions. This framework provides physical insights into excited state lifetimes, charge separation dynamics, and dipole moments across diverse DNA sequences. By integrating quantum physics and physical chemistry methodologies with genetic and epigenetic analyses, this study offers a powerful interdisciplinary approach to investigate the quantum mechanisms underlying DNA charge dynamics and their modulation by epigenetic modifications.

BP 17.66 Tue 18:00 P4

Modeling host-pathogen interactions: infection process as a population dynamics problem — •Soham Mukhopadhyay[1], Jonathan Pollock[2], David Voehringer[2], and Vasily Zaburdaev[1] — [1]Department of Biology, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Department of Infection Biology, Uniklinikum Erlangen, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Helminth infections affect a large proportion of the world's population and cause significant morbidity. There are no vaccines against helminths, and the mechanisms by which the body fights off helminth infections are not well-understood. To better understand the immune system response we aim to develop a mathematical model describing the helminth load in different organs of the host as a function of time. As an experimental system, we use murine helminth infection by *Nippostrongylus brasiliensis*. We abstract infection progression as a state-transition process. The different host organs involved in the infection cycle act as the different states of the system, and the worms are treated as identical and independent particles transitioning from one state to another with fixed transition rates and delays. This allows simulation of the infection process via kinetic Monte Carlo and association of the infective dose of larvae to the number of eggs shed to the environment by adult worms from the intestine, which can then be compared against experimental data. Using simulations to generate training data, we employ Neural Network-based optimization to discover an optimal parameter set that can quantify the infection process.

BP 17.67 Tue 18:00 P4

Measuring activity from particle trajectories — •Lukas Abegg, Till M. Muenker, and Timo Betz — Third Institute of Physics, Georg August Universität Göttingen, Göttingen, Germany

Is it possible to distinguish activity from thermal fluctuations just from observed trajectories? The newly introduced statistical quantity Mean Back Relaxation aims to achieve exactly this by using three-point correlation functions. This non-dimensional function yields a measure for deviation from equilibrium within a confined system. It is calculated as the average displacement of a tracer article under the condition of having moved the distance d in advance. For an equilibrium process, this quantity results in a long time value of $\frac{1}{2}$. However, deviation from this value is a marker for broken detailed balance. To gain deeper insight into this new statistical measure, we investigate this quantity inside a controlled system, namely a viscoelastic polyacrylamide gel. This probe was tuned to imitate the mechanical properties of cells, containing polystyrene particles with a size of one micron. To drive this system out of equilibrium, we use a movable optical tweezer to simulate active motion of the particle. The Mean Back Relaxation is calculated for all trajectories and fitted with an analytical solution for a viscoelastic system. The results are used to quantify the diffusion coefficient of the trapping laser and thus, the activity of the system tuned by our experimental realisation. Additionally, we can calculate the shear modulus $G^\star$ from this result.

BP 17.68 Tue 18:00 P4

Active Soft Glassy Rheology as a model for cytoskeletal mechanics — •Raffaele Mendozza and Peter Sollich — University of Goettingen, Institute for Theoretical Physics

The cytoskeleton plays a vital role in cellular processes like growth, migration, and division, owing to its unique mechanical properties [1]. Advanced microrheology techniques have revealed a complex power-law viscoelastic spectrum in this and other biopolymer networks, reflecting the presence of a broad distribution of relaxation timescales [2]. Coarse-grained trap models capture this phenomenology, suggesting a connection between cytoskeletal and soft glassy rheology (SGR) [3,4,5]; however, the original SGR model lacks explicit consideration of active processes, ubiquitous in living cells. We therefore explore how activity influences the rheological response of a soft glassy material, based on different working hypotheses. By introducing an activity-dependent effective temperature, the characteristic SGR viscoelastic spectrum is recovered, while modelling activity as an effective strain rate introduces a competing timescale that modifies the response. The resulting active SGR model provides insights into the mechanical behavior of cells independent of biochemical intricacies, serving as a foundation for future models incorporating more detailed structural information.

[1] P. Kollmannsberger and B. Fabry, 2011
[2] B. Fabry et al., 2001
[3] B. D. Hoffman1 and J. C. Crocker, 2009
[4] K. K. Mandadapu et al, 2008
[5] P. Sollich et al, 1997

BP 17.69 Tue 18:00 P4

Fluctuating liquid inclusions morphology in biomolecular condensates driven by fuel-dependent binding agents — •Leonardo Silva-Dias and Christoph A. Weber — Universität Augsburg, Augsburg, Germany

The presence of aggregation-prone proteins in non-dilute, multi-component solutions, such as the cellular environment, can lead to the formation of protein aggregates. In these environments, such proteins may also undergo phase separation, forming biomolecular condensates. Both processes are regulated by specialized molecules known as binding agents, examples of which include RNA, enzymes, and chaperones. These binding agents continuously consume biological fuels, driving the system out of equilibrium and enabling the emergence of complex behaviors, such as morphological changes in the condensates. Specifically, recent experimental evidence has shown that a system composed of aggregation-prone proteins and ATP-driven chaperones induces the formation of condensates with a fluctuating liquid inclusions morphology. Based on these observations, the present work provides a theoretical framework to describe the emergence of the fluctuating liquid inclusions state. The proposed description is developed through a mean-field model that accounts for chemical reactions and phase separation in the presence of stochastic fluctuations. In this system, we observed that local fluctuations trigger multiple nucleation events within the condensates, leading to the growth of many liquid inclusion structures, which ripen, dissolve, and renucleate.

BP 17.70 Tue 18:00 P4

Competitive resource sharing mechanism for synchronization and its energy cost — •Dongliang Zhang[1,2], Yuansheng Cao[1], Qi Ouyang[3], and Yuhai Tu[4] — [1]Department of Physics, Tsinghua University, Beijing, China — [2]Max Planck Institute for the Physics of Complex Systems — [3]School of Physics, Zhejiang University, Hangzhou, China — [4]IBM T. J. Watson Research Center, Yorktown Heights, New York, USA

Synchronization among a group of active agents is ubiquitous in nature. Although synchronization mechanism based on direct pairwise interactions between agents as exemplified by the Kuramoto model is well understood. The dynamics and energetics of another general mechanism based on indirect interactions among agents sharing a limited resource are less known. In this work, we proposed a simple thermodynamically consistent model for the resource-sharing (RS) mechanism.We find that synchronization relies on differential competence of agents for the limited resources.More advanced agents are less competent, which provides a negative feedback mechanism resulting in synchronization. We show that differential affinity breaks detailed balance and thus synchronization requires continuous energy dissipation in addition to the energy cost of the agents* processive motion. Our study reveals a tradeoff relation between the total energy dissipation rate and the performance of the system characterized by its average speed and synchronization accuracy. Different Pareto fronts with fixed dissipation or speed result naturally from the Energy-Speed-Accuracy (ESA) relationship.

BP 17.71 Tue 18:00 P4

Time irreversibility and effective temperature are independently regulated in the actin cortex of living cells — •N Narinder and Elisabeth Fischer-Friedrich — Cluster of Excellence Physics of Life, Technische Universität Dresden, Dresden, Germany

Living cells exhibit non-equilibrium dynamics driven by the intricate interplay between motor activity and their viscoelastic environment. The deviation from thermal equilibrium termed as irreversiblity is commonly characterized by an increased effective temperature and time-reversal symmetry breaking quantified through the Kullback-Leibler divergence (KLD). In this study, we determine entropy production as

a measure of irreversibility both by the effective temperature and the KLD in the actin cortex of living cells using atomic force microscopy (AFM) with and without pharmacological treatments that modulate cellular activity and cortical mechanics. Surprisingly, we find that while the entropy production rate consistently increases with effective temperature, its time irreversibility estimated by the KLD can exhibit an opposite trend, depending on the mechanical properties of the cortex. Our findings underpin the role of mechanical properties on the irreversibility. Further, the findings are supported by a minimal model of the AFM tip as probe immersed in the viscoelastic environment of active cell cortex.

BP 17.72 Tue 18:00 P4

Triacylglycerols affect the water content and cohesive strength of collagen fibrils — •Martin Dehnert, Tiberius Klose, Yang Pan, Dietrich R. T. Zahn, Maximilian Voigtländer, Johannes F. Teichert, and Robert Magerle — Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany

Collagens, lipids, and water are among the major molecular components of connective tissue, but surprisingly little is known about their interactions in vivo. Here, we provide direct evidence that type I collagen fibrils extracted from chicken calcaneal tendon contain triacylglycerols (TAG), which influence the water content of the fibrils and act as plasticizers that affect the mechanical properties of the fibrils. We use organic solvents to dissolve lipids from native collagen fibrils and identify them as TAG using Raman spectroscopy and NMR spectroscopy. Using atomic force microscopy-based 3D depth profiling, we quantify the changes in volume, water content, and indentation modulus of the fibrils caused by the removal of TAG at the single fibril level. Based on these findings, we propose a molecular model for the intercalation of TAG into collagen fibrils. The discovery of the biomechanical function of TAG is fundamental to understanding the role of lipids in collagen fibrils during development, aging, and disease.

BP 17.73 Tue 18:00 P4

Cellular Potts Model links tissue surface tension to cell proliferation — •Kai Lennard Fastabend[1], Cécile M. Bidan[2], John W. C. Dunlop[3], and Philip Kollmannsberger[1] — [1]Biomedical Physics, Heinrich Heine University Düsseldorf, 40225 Düsseldorf, Germany — [2]Max Planck Institute of Colloids and Interfaces, Dept. of Biomaterials, Golm, Germany — [3]Paris Lodron University, Salzburg, Austria

The shape and growth kinetics of tissue depend not only on biochemical factors but also on the geometry of the extracellular environment. Cellular Potts Model simulations of tissue growth on different substrate geometries are a promising approach to investigate the role of adhesion forces, cell elasticity and tissue surface tension in the formation and organisation of tissue. To investigate how tension-dependent cell proliferation in tissues can explain the observed link between scaffold geometry and tissue growth kinetics, we implemented a growth rule based on the stretching of cells in CompuCell3D. Systematic parameter scans reveal the role of cell-substrate adhesion as the driving factor for monolayer formation, while cortical contractility introduces a surface tension to the tissue. The minimization of the macroscopic tissue surface leads to bulk tissue growth beyond the monolayer depending on the underlying substrate geometry. Our results highlight how cellular contractility and adhesion, together with geometric boundary conditions can determine the macroscopic growth patterns of tissues, independent of soluble growth factors.

BP 17.74 Tue 18:00 P4

Nanomechanical ultrastructure of native tendon tissue — Mario Zerson, Martin Dehnert, Paul Zech, Tiberius Klose, and •Robert Magerle — Fakultät für Naturwissenschaften, TU Chemnitz

Tendon tissue is a natural, high performance material in which type I collagen fibrils act as the load-bearing elements. The collagen fibrils are embedded in the tendon ground substance, a hydrophilic gel. Using AFM-based nanoindentation measurements, we study the nanomechanical ultrastructure of collagen fibrils in native tendon tissue obtained from the calcaneus (Achilles) tendon of chicken. The sample is exposed to a flow of humid air with controlled relative humidity to maintain the water content close to physiological conditions. We reconstruct 3D depth profiles from measured force–distance data and analyze the tip–sample interaction with a recently developed hysteresis model with return point memory (Soft Matter 2024, *20*, 2831–2839). The latter describes the rate-independent nanoindentation response, which is dominated by an elasto-plastic deformation behavior. It allows us to quantify the elastic and dissipative contributions of the indentation response within individual collagen fibrils as well as in the contact regions between adjacent fibrils.

BP 17.75 Tue 18:00 P4

Adjustable tension in reconstituted heart muscle tissue to mimic physiological mechanical environment changes — •Anna Mukhina[1], Till Muenker[1], Mattias Luber[1], Arne Hofemeier[2], Bruno Schmelz[1], and Timo Betz[1] — [1]Third Institute of Physics - Biophysics, University of Goettingen — [2]Department of Pharmacology and Toxicology, University Medical Center Goettingen

The development of in vitro 3D muscle tissues is critical for studying muscle physiology, disease mechanisms, and drug responses. PMMA tissue chambers provide structural support for myogenic cells embedded in a 3D ECM scaffold, enabling organization into aligned myotubes resembling natural muscle tissue. Tissue self-organizes around posts of known stiffness, with muscle strength assessed via post-deflection during contraction. This project introduces a piezo-driven actuator into the PMMA chamber for external manipulation of tissue tension. Combining actuators with a direct readout of posts' positions enables feedback control to emulate diverse mechanical environments. This innovation investigates how varying mechanical loads influence muscle development, adaptation, and therapeutic responses.

The project involves: (1) design and integration of a piezo actuator system, using CAD and Labview for construction and feedback control; (2) validating the modified chamber with engineered human myocardium (EHM) derived from iPSCs, exposed to defined mechanical stresses to mimic physiological and pathological loads. Functional and morphological outcomes are assessed via post deflection analysis and fluorescence imaging, advancing insights into muscle biomechanics.

BP 17.76 Tue 18:00 P4

Illuminating forces in living tissues — •Lucia Baldauf[1], Anna Bajur[2], Katelyn Spillane[2], and Guillaume Charras[1] — [1]London Centre for Nanotechnology, University College London, UK — [2]Department of Life Sciences, Imperial College London, UK

How can epithelial tissues withstand large forces and support deformations that drastically increase their length? Adult epithelial tissues regularly experience forces that stretch them by up to 50 %, and deformations can reach several hundred percent during development. To fulfill their physiological barrier function, epithelia must accommodate such large deformations without fracturing. Consequently, cell-cell adhesions must be finely tuned, or pathologies like skin blistering or cancer metastasis can occur. However, the physical principles governing tissue integrity remain difficult to study, since tissue fracture is a multiscale process spanning up to 10 orders of magnitude in both size and force. Millimetre-sized tissues can withstand millinewton-forces, but tissue fracture results from the local failure of single nanometre-sized adhesion complexes that bear piconewton forces. New tools are needed to bridge these vastly different scales and understand what molecular processes lead to tissue failure. Here we develop a new experimental tool to study tissue integrity and force propagation across scales. We engineer living model tissues where DNA-based molecular force sensors in chimeric cell-cell junctions provide a local molecular-scale force readout, for the first time illuminating how forces propagate in living tissues under stretch.

BP 17.77 Tue 18:00 P4

Imaging cell mechanics of retina organoids using an oblique plane light-sheet microscope — •Achim Theo Brinkop[1,2], Florian Schorre[1], Stefan Stöberl[1], Elijah R. Shelton[1], Teresa Rogler[1,2], Michael Frischmann[1,2], Marie Lackmann[1], Kaustav Goswami[1], Alexander Zangl[1], Mythili Padavu[1], and Friedhelm Serwane[1,2,3] — [1]Faculty of Physics & Center for NanoScience, LMU Munich, Germany — [2]Institute of Biophysics, Ulm University, Germany — [3]Munich Cluster for Systems Neurology (SyNergy) & Graduate School of Systemic Neuroscience (GSN), Munich, Germany

Retina organoids have become a powerful testbed for studying retina formation and neuronal development. Our current measurements of the creep compliance in retina organoids with magnetic droplets point towards soft glassy rheology of developing retinal tissue at second to hour timescales. As a next step, we explore whether the motion of cells agrees with predictions for glassy materials. For this purpose, we built a custom oblique plane microscope for long-term volumetric imaging of the cell movements during organoid development. Using a processing pipeline based on open-source python packages (Cellpose3, Ultrack),

we segment and track individual cells. The tracks allow us to quantify cell dynamics and compare these with existing models for glassy materials. In the future, we will integrate magnetic droplet compliance measurements with volumetric imaging in one set-up to simultaneously probe organoid mechanics *in situ*. Combining tissue mechanics measurements with cell dynamic recordings, we aim to shed light on the mechanical cues that guide retina formation.

BP 17.78 Tue 18:00 P4

Investigating the mechanosensitive expression of sema3A and slit1 in hydrogel-embedded neuroepithelial cells — •Niklas Gampl[1,2] and Kristian Franze[1,2,3] — [1]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [2]Institute of Medical Physics and Microtissue Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [3]Department of Physiology, Development and Neuroscience, University of Cambridge, Cambridge, UK

During brain development, neurons extend long axons that grow along well-defined pathways to their destination. This axon pathfinding is regulated by chemical guidance cues, which are produced by neuroepithelial cells, and by tissue stiffness. To investigate whether environmental stiffness regulates the expression of chemical guidance cues in the developing brain, we developed a framework to culture Xenopus tissue explants in collagen-based hydrogels with tunable stiffness. We found an increase in sema3A and slit1 mRNA levels in hypothalamic neuroepithelial tissue cultured in stiff hydrogels (G' = 450 Pa) compared to soft hydrogels (G' = 40 Pa). Additionally, 3D traction force microscopy revealed that strain energy, generated by the explants and stored in the matrix, increased with stiffness. These findings highlight a mechanochemical mechanism linking tissue stiffness to chemical guidance cue expression. Further investigation could improve our understanding of the complex interplay between guidance cues and their integration by cells.

BP 17.79 Tue 18:00 P4

AFM imaging of epithelial basement membrane with and without molecular perturbations — •Karla Yanin Guerra Santillan[1], Christian Dahmann[2], and Elisabeth Fischer-Friedrich[1] — [1]Cluster of Excellence Physics of Life, Technische Universit\"at Dresden, Dresden, Germany — [2]School of Science, Technische Universit\"at Dresden, Dresden, Germany

Understanding the precise regulation of growth and form is fundamental to the healthy development of all organisms. The basement membrane is a specialized sheet of extracellular matrix that forms at the basal face of epithelial tissues. This biopolymer network plays a major role in structural support, proliferation regulation and biochemical signalling. Here, we present data of high-resolution images of the basement membrane in developing wing discs of the fruit fly Drosophila melanogaster using atomic force microscopy. We find that depending on the developmental stage, micron-sized ripple patterns of different amplitude are present on the surface of the basement membrane that depend on the presence of individual ECM proteins.

BP 17.80 Tue 18:00 P4

Species-specific biomineral pattern formation in centric diatoms — •Francesco Leone[1], Nils Kröger[1,2], and Benjamin M. Friedrich[1] — [1]Physics of Life, TU Dresden, 01307 Dresden — [2]B CUBE, TU Dresden, 01307 Dresden

Diatoms are unicellular algae known for their intricately patterned cell walls, primarily composed of amorphous silica (SiO2). Their hierarchically patterns biomineral architectures display outstanding material properties but also represent an ideal model system to study species-specific pattern formation during biomineralization by living organisms. In centric "barrel-shaped" diatoms, the "lids" display three prominent pattern features: branched rib patterns with radial symmetry, nano-pores and transverse connections. How these different pattern features evolve and mutually influence each other is not known. We are extending a mathematical model of branching morphogenesis, previously developed in our group for a single model species [1], to account for the variety of patterns in related species and mutants. To facilitate a rigorous quantitative comparison to electron microscopy images, we are developing automated image analysis pipelines for the morphometric characterization of different phenotypes. Through this research, we aim to reverse-engineer putative chemical and physical mechanisms taking place during diatom silica cell wall formation.

[1] Babenko et al. PNAS 121(10): e2309518121 2024

BP 17.81 Tue 18:00 P4

Self-stimulated growth of epithelial model tissues — •Maja Milas[1], Damir Vurnek[2], Narmin Abasova[2], Kevin Höllring[2], and Ana-Sunčana Smith[1,2] — [1]Group for Computational Life Sciences, Division of Physical Chemistry, Ruđer Bošković, Institute, Zagreb, Croatia — [2]PULS Group, Center for Advanced Materials and Processes, FAU Erlangen-Nürnberg

The growth of epithelium is one of the fundamental biological processes required for sustaining the life of multicellular organisms. This process can be studied in appreciable detail using model systems such as radially growing 2D MDCK colonies. Typically, epithelium grows from low densities to the homeostatic state while expanding laterally. This process has, in the past, been captured using Fisher Kolmogorov-like growth laws, where shortly after the establishment of homeostasis, the moving front reaches a constant velocity and density profile. However, in experiments presented herein, we show that the moving front continues to accelerate and expand for days after the steady state density is achieved in the center of the colony. This radial expansion cannot be captured by currently established models, even after introducing a highly non-linear growth term and recently proposed delays. We can, nonetheless, rationalize this growth scenario by introducing self-stimulation by an activator secreted and absorbed in a density-dependent manner and coupling it with the equation for the evolution of the density. Further work is necessary to identify the biochemical pathway regulating the effect of the activator.

BP 17.82 Tue 18:00 P4

Epithelial Tissue Response Under Solid Shear Stress — •Narmin Abasova[1], Annemarie Wirth[1], Kevin Hoellring[1], Rudolf Merkel[2], and Ana-Sunčana Smith[1,3] — [1]PULS Group, Institute for Theoretical Physics, FAU Erlangen- Nurnberg (IZNF) — [2]Institute for Biological Information Processes (IBI), Forschungszentrum, 52428 Jülich, Germany — [3]Group of Computational Life Sciences, Division of Physical Chemistry, Ruder Bošković Institute, 10000 Zagreb, Croatia

Epithelial cells are subjected to a diverse range of mechanical stresses in the human body, from the dynamic forces generated during physical activity to the rhythmic pulsations of blood flow. To better understand the mechanobiological processes due to various stress types, it is essential to investigate how they influence cellular responses and tissue functionality. Among the different forms of mechanical stress, solid shear stress transmitted through the extracellular matrix (ECM) remains a relatively underexplored side of tissue mechanics. Our research addresses this gap by utilising a custom-designed device that applies controlled shear stress to the substrate supporting epithelial cell cultures. By subjecting targeted cell clusters to solid shear stress, we observe and document the tissue's behavior under a microscope. This study examines key aspects of cellular response, including stress relaxation, proliferation, morphological alterations and topological changes at cell membranes, where neighboring cells exchange positions. Using stress-generating devices in this context allows us to better understand how distinct stress types influence tissue behavior.

BP 18: Tissue Mechanics

Time: Wednesday 9:30–13:00 Location: H44

Invited Talk BP 18.1 Wed 9:30 H44

Mechanical Imprints of Cell Competition — •Benoit Ladoux — Institut Jacques Monod, Université Paris Cité & CNRS

Epithelial tissues are dynamic communities of cells characterized by close intercellular communication and highly coordinated motion. The mechanical properties of these tissues are crucial for understanding key biological processes, such as homeostasis, morphogenesis, and metastasis, and are tightly regulated through cell-cell interactions. In this presentation, I will explore the role of mechanical forces in cell competition - a process where the expansion of one cell population drives the elimination of another. I will demonstrate how intercellular force transmission governs this competitive interaction, shedding light on the interplay between mechanics and cellular mechanisms.

BP 18.2 Wed 10:00 H44

Regulation of Homeostatic Tissue Composition and Self-Organization via Pressure-mediated Cell Cycle Control in Stem Cell-Derived Epithelial Tissues — •Johannes Krämer[1], Edouard Hannezo[2], Gerhard Gompper[1], and Jens Elgeti[1] — [1]Forschungszentrum Jülich, Institute for Advanced Simulations — [2]Institute of Science and Technology Austria

Tissue homeostasis relies on a precise balance between cellular proliferation and differentiation, with spatial cell distribution playing a critical role in effective replenishment. The mechanisms governing self-renewing cell types, including their proliferation rates, mechanical interactions, and spatial organization, remain incompletely understood. Here, we present a study of epithelial tissue dynamics using a descendant lineage model derived from slow-cycling, self-renewing stem cells. Through mean-field analysis, we establish conditions for cell cycle parameters that maintain a well-defined tissue configuration and demonstrate the influence of mechanical regulation on division control. To further explore spatio-temporal properties, we implement the lineage model in an agent-based computational framework, incorporating cell-cell mechanical interactions. Our findings reveal a regime in which stem cells exhibit long-range order, forming small, localized niche-like clusters with slow diffusion. These insights offer a novel perspective on the interplay between proliferation, differentiation, and the role of mechanical interactions on the spatial organization of cells, advancing our understanding of tissue homeostasis.

BP 18.3 Wed 10:15 H44

Spatiotemporal Analysis of Active Deformation of Patient-derived Colon Cnacer — •Shogo Nagai[1], Ryo Suzuki[2], Go Yamakawa[3], Akihisa Fukuda[3], Hiroshi Seno[3], and Motomu Tanaka[1,4] — [1]Physical Chemistry of Biosystems, Heidelberg University, Heidelberg, Germany — [2]Department of Biosciences and Informatics, Keio University, Tokyo, Japan — [3]Department of Gastroenterology and Hepatology, Kyoto University Graduate School of Medicine, Kyoto, Japan — [4]Center for Integrative Medicine and Physics, Kyoto University, Kyoto, Japan

Biomedical cancer research has relied on the investigation of fixed cells and tissues, in which the non-equilibrium dynamics of cancer have been largely overlooked. Extending the recent studies shedding light on the dynamics of the isolated cells, spatiotemporal analysis of cancer on a multicellular level is expected to reveal the dynamic mechanisms of cancer progression.

In this study, the time evolution of active deformation of growing colorectal cancer organoids (miniaturized organ model) was quantitatively evaluated by the Fourier expansion. Thereby, the larger deformation of malignant genetic mutated organoids was extracted, which was attributed to the slow effective viscoelastic relaxation. The simulation of the double-cell stage indicated the characteristic dynamics of organoids could be related to cell-cell junctions. In addition, biomedical evaluations showed lower cell-cell junctions of malignant colorectal cancer on a protein and RNA level.

BP 18.4 Wed 10:30 H44

a novel 3D platform for investigating cancer cell migration and tissue organization under mechanical load — •Mattias Luber, Bruno Schmelz, Mahboubeh Farajian, and Timo Betz — Third Institute of Physics - University of Göttingen - Germany

Recent advances in tissue engineering and mechanobiology have highlighted the critical role of mechanical forces in guiding cellular organization and extracellular matrix (ECM) remodeling. Building on these findings, we introduce a novel platform for engineering connective tissues that facilitates high-resolution live imaging of self-organization and ECM remodeling under diverse experimental conditions. This platform employs controlled mechanical loading to induce fibroblast alignment, resulting in the formation of highly organized tissue structures. By enabling both global and localized measurements of tissue tension and providing precise control over mechanical load, it allows for the detailed investigation of ECM remodeling, cellular dynamics, and nuclear deformation. A key application of this platform is in uncovering how mechanical properties of the tissue environment influence cancer cell behavior. By integrating models of MDA-MB-231 breast cancer cells, we demonstrated how variations in tissue tension and ECM structure directly modulate cancer cell migration patterns. These findings highlight the critical interplay between mechanical forces and cellular invasiveness, providing insights into the biomechanical drivers of cancer progression.

BP 18.5 Wed 10:45 H44

Bridging the gap between single cell and tissue mechanics — •Mathilde G. Lettinga[1], Antje Garside[1], Vaibhav Mahajan[1], Franziska Baenke[2], Valeria Lozovanu[2], Daniel Stange[2], Ingolf Sack[3], and Anna V. Taubenberger[1] — [1]Center for Molecular and Cellular Bioengineering (CMCB), BIOTEC, Dresden University of Technology, Germany — [2]Department of Visceral, Thoracic and Vascular Surgery, University Hospital Dresden, Germany — [3]Department of Radiology, Charité - Universitätsmedizin Berlin, Germany

Tumours exhibit altered biophysical properties across spatial scales. Compared to healthy tissue, solid tumours are typically stiffer, while individual cancer cells are more compliant. The increased tissue stiffness can partly be attributed to the extracellular matrix. However, the contributions of single cell mechanics and collective cell behaviour to the emergent tissue properties remain unclear.

To bridge this gap between single cell and tissue mechanics, we have established a 3D in vitro tumour model, based on patient-derived colorectal liver metastasis organoids grown in hydrogels mimicking the extracellular matrix. Cells retrieved from dissociated organoids were mechanically characterised with real-time deformability cytometry and AFM. These data were benchmarked to the morphometric and mechanical properties of intact organoids, which were assessed in situ by confocal and Brillouin microscopy. The bulk mechanical properties of our model system were investigated using tabletop magnetic resonance elastography. Our data contribute to a better understanding of the mechanical coupling between single cells and tissues.

BP 18.6 Wed 11:00 H44

Exploring glassy dynamics in retina organoids through time-series imaging — •Alexander Johann Zangl[1], Achim Theo Brinkop[1,2], Elijah R. Shelton[1], Marie Lackmann[1,2], Teresa Rogler[1,2], and Friedhelm Serwane[1,2,3] — [1]Faculty of Physics & Center for NanoScience, LMU Munich, Germany — [2]Institute of Biophysics, Ulm University, Ulm, Germany — [3]Munich Cluster for Systems Neurology (SyNergy) & Graduate School of Systemic Neuroscience (GSN), Munich, Germany

Quantifying cell dynamics and the mechanical forces guiding such movements can provide crucial insights for understanding tissue development and disease progression. Stem cell derived neuronal organoids provide an accessible system for studying nervous tissue development in the laboratory. Recently, magnetic droplet based mechanical measurements in retina organoids revealed a weak power-law scaling in the mechanical properties, suggesting that the retinal tissue is a glassy material. While the mechanical observations are consistent with predictions of soft glassy rheology, whether the movements of the individual cells making up those tissues are also in agreement with a glassy material is still unknown. Using confocal fluorescent time-series imaging, we observe the movements of nuclei in the forming retina. By tracking cells, we can determine whether cellular movements also point to the retina as a solid-like material just above a glass transition. We characterize the cell dynamics of the tissue by analysing the scaling of the mean-square displacements of the nuclei. This will help us understand how mechanical cues guide retina formation.

15 min. break

BP 18.7 Wed 11:30 H44

Statistical Inference and Selection of a Mechanistic Model during Tissue Specification in Beetle Embryogenesis — •Zoë Lange[1,2], Franziska Krämer[3], Frederic Strobl[3], Ernst H.K. Stelzer[3], and Franziska Matthäus[1,4] — [1]Frankfurt Institute for Advanced Studies — [2]Fachbereich Physik, Universität Frankfurt am Main — [3]Buchmann Institute for Molecular Life Sciences — [4]Fachbereich Informatik und Mathematik, Universität Frankfurt am Main

During development of the beetle Tribolium castaneum, the blastoderm differentiates into embryo and extra-embryonic serosa tissues with distinct morphologies. Using statistical inference, we estimate effective cell tensions and pressures based on cell geometry and a force-balance assumption. Our analysis reveals an inverse relationship between tension and cell shape with characteristic slopes for serosa and embryo tissues. We identify and parametrize a mechanistic vertex model that captures the differing properties of serosa and embryo cells. This study demonstrates how statistical inference can guide the selection and refinement of mechanistic models to understand tissue dynamics during embryogenesis.

BP 18.8 Wed 11:45 H44

Dynamics and mechanics of germband extension in *Drosophila* — •Maryam Setoudeh[1,2,3], Giulia Serafini[3], Pavel Tomancak[3,4], and Pierre A. Haas[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Center for Systems Biology Dresden — [3]Max Planck Institute of Molecular Cell Biology and Genetics — [4]Cluster of Excellence Physics of Life, TU Dresden

During *Drosophila* development, cell intercalations and cell divisions drive the extension of the germband on the dorsal side of the embryo towards its anterior. We and others [1] have recently observed that the shape of the germband is often curved, even in the wild-type, contrary to the textbook picture of a straight germband. Here, we develop a mechanical model in which the germband midline appears as an elastic line pushed by an effective force resulting from germband extension. Its motion is resisted by frictional forces from surrounding tissues and attachment at the tip mediated by the integrin scab. In this model, we discover an instability of the straight shape that explains the observed variability in the wild-type as well as the twisting phenotype observed in embryos in which scab is depleted. We also find that an alternative model of a growing rather than pushed elastic line cannot explain the observed instability. This highlights the mechanical role of these pushing forces in germband extension.

[1] Smits *et al.*, Curr. Biol. **33**, 3536 (2023)

BP 18.9 Wed 12:00 H44

A mechanical model of the symmetry breaking of the shape of the primordial hindgut — Daniel S. Alber[1,2], Shiheng Zhao[3,4,5], Eric F. Wieschaus[2,6], Stanislav Y. Shvartsman[2,6,7], and •Pierre A. Haas[3,4,5] — [1]Department of Chemical and Biological Engineering, Princeton University — [2]Lewis-Sigler Institute for Integrative Genomics, Princeton University — [3]Max Planck Institute for the Physics of Complex Systems — [4]Max Planck Institute of Molecular Cell Biology and Genetics — [5]Center for Systems Biology Dresden — [6]Department of Molecular Biology, Princeton University — [7]Center for Computational Biology, Flatiron Institute

During early *Drosophila* morphogenesis, as the germband extends and the midgut invaginates, the initially circular primordial hindgut moves from the posterior pole of the embryo to its dorsal side and folds into a characteristic keyhole shape. Here, we develop a minimal model of this symmetry breaking in which the hindgut appears as an inextensible elastic ring in the plane. We discover that, as the area enclosed by the ring decreases (midgut invagination) while a diameter is held fixed (germband extension), the circular shape bifurcates robustly into the observed keyhole shape. Moreover, we show how embryonic curvature breaks symmetry further to select the observed orientation of the keyhole shape. This demonstrates that morphogenesis of the primordial hindgut can be a passive mechanical consequence of active deformations of the tissues that surround it.

BP 18.10 Wed 12:15 H44

What mouse embryos can teach us about tissue spreading — •María-José Franco-Oñate[1], Ricard Alert[1], and Kate Cavanaugh[2] — [1]MPI for the Physics of Complex Systems, Dresden, Germany — [2]University of San Francisco in California, United States

Processes such as embryogenesis, tissue repair and cancer metastasis are dependent upon the migration of large groups of cells through changes in group morphogenesis or collective migration. These processes entail both molecular and mechanical interactions between cells and their surrounding environment. Several attempts have been made to create models of these interactions [1].

In this study, we focus our attention on mouse embryos during implantation. In this process, the embryo adheres to the substrate and extends along it. The results of ongoing experiments indicate that embryos derived from older mice are unable to implant, resulting in a lack of spreading of the tissue that adheres to the substrate. The objective of this study is to gain insight into the mechanisms underlying the spreading process and its dependence on the age of the embryo. To this end, we employ a coarse-grained approach, in which the tissue is conceptualised as an active polar fluid, to investigate the dynamics of a spreading tissue [2]. To validate our theoretical model, we utilise traction force microscopy, which enables us to quantify the forces exerted by the tissue.

[1] R. Alert and X. Trepat. Ann. Rev. 11: 77-LF1 (2020)
[2] C. Pérez-González, R. Alert, et al. Nat. Phys. 15: 79-88 (2019)

BP 18.11 Wed 12:30 H44

Growth control in development and regeneration in the zebrafish pectoral fin — •Maximilian Kotz[1,2], Lucas de Oliveira Petrocchi Ribas[1,3], Shivani G. Ramkumar[1,3], Rita Mateus[1,3], and Benjamin M. Friedrich[1,2] — [1]PoL, Dresden, Germany — [2]cfaed, Dresden, Germany — [3]MPI-CBG, Dresden, Germany

Although all multicellular organisms can develop from a single cell, only few organism can regenerate lost body parts in adulthood. If it as an open question whether the mechanisms controlling growth in regeneration are the same as those in development. We combine theory and experiment to address this question using the pectoral fin of zebrafish as a model system. As a novel paradigm, we compare unperturbed development and regeneration after partial amputation during development. To quantify growth, we developed machine learning-based image analysis pipelines and introduce a curvilinear coordinate system to describe the geometry of the tissue. Tissue samples from different individuals became comparable by defining diffeomorphisms that minimize an elastic pseudo-energy, which enables a rigorous statistical comparison of proliferation rates, shape changes and even morphogen gradients. This quantification revealed that volume growth is driven by distinct processes. In particular, growth along the different body axes is markedly different, with thickness growth apparently uncoupled from in-plane growth. To identify the underlying mechanisms of growth control, we probe predictions from different mathematical models by investigating different amputation scenarios, along with genetic or pharmacological perturbations.

BP 18.12 Wed 12:45 H44

Model of growth arrests and proportional growth inspired by axolotl limb regeneration — •Natalia Lyubaykina[1,2], Dunja Knapp[3], Pietro Tardivo[4], Tatiana Sandoval-Guzmán[3], Elly Tanaka[4], and Benjamin M Friedrich[1,2] — [1]Cluster of Excellence 'Physics of Life', Technical University Dresden, Dresden, Germany — [2]Center for Advancing Electronics, Technical University Dresden, Dresden, Germany — [3]CRTD/Center for Regenerative Therapies TU Dresden, Germany — [4]Research Institute of Molecular Pathology, Vienna Biocenter (VBC), Campus Vienna Biocenter, Vienna, Austria

Axolotl can regenerate lost limbs even as adults, posing the question of how the size of a regenerating limb is matched to a variable animal size. Two interacting morphogens, SHH and FGF8, regulate limb development and regeneration. Inspired by this biological example, we theoretically investigate general mechanisms of morphogen-controlled growth arrest and proportional growth. In the proposed model, tissue growth increases the spatial distance between both morphogen gradients, thus providing negative feedback that eventually arrests growth. We propose two distinct scaling scenarios of morphogen gradients: either dynamic scaling with regenerating blastema size, or static scaling with animal size. We show that only the latter ensures robust growth arrest and proportional growth. We compare theory predictions to experimental quantification of SHH and FGF8 dynamics at different time points of regeneration in different-sized animals, suggestive of scaling with animal size.

BP 19: Membranes and Vesicles II

Time: Wednesday 9:30–13:00 Location: H46

BP 19.1 Wed 9:30 H46

Atomistic Insights into pH-Dependent Structural Transitions in Lipid Mesophases: A Combined MD/SAXS Approach — •Akhil Sudarsan[1], Julian Philipp[2], Joachim Rädler[2], and Nadine Schwierz[1] — [1]University of Augsburg, Augsburg, Germany — [2]Ludwig Maximilians-University, Munich, Germany

Lipid nanoparticles (LNPs) are crucial delivery vehicles for mRNA-based therapeutics, enabling the encapsulation and release of negatively charged nucleic acids through ionizable lipids that exhibit pH-dependent fusogenic activity. This study investigates ionizable DLin-MC3-DMA (MC3) lipid/cholesterol mesophases that mimic the core structure of LNPs, focusing on the inverse hexagonal (H_{II}) and inverse micellar (L_{II}) phases, both featuring an internal water domain surrounded by ionizable lipids. By combining experimental SAXS data and molecular dynamics (MD) simulations, we show that the L_{II} phase, which is stable at higher pH, transitions to H_{II} at lower pH. We also calculate the water content of the simulated core phases through comparison with scattering data and elucidate the distribution of lipids in these mesophases. We further developed an approach to compute scattering profiles directly from MD simulations, which corrects for artifacts arising from periodic boundary conditions, enabling direct, model-free comparisons between experimental and simulated data enhancing the reliability of the structural interpretations. In summary, integrating SAXS experiments and MD simulations offer molecular insights into the dynamic behaviour and pH-dependent structural transitions of ionizable lipid mesophases.

BP 19.2 Wed 9:45 H46

The effect of long-chain sphingolipids on lipid bilayers — •Clara Rickhoff, Annemarie Quas, and Andreas Heuer — Institut für Physikalische Chemie, Universität Münster, Münster, Germany

Lipid bilayers are found to form microdomains, so called rafts, that support a sorting of compounds in the bilayer, and that way are thought to be essential for cellular processes, such as vesicular traffic. One type of raft that is found in lipid bilayers of e.g. yeast cells in experiments are sphingolipid-enriched and sterol-depleted domains, that seem to form gel-like domains. In our work, we conduct MD simulations of lipid bilayers containing different concentrations of long-chain sphingolipids in order to investigate their effect on the membrane at the atomistic level. The remaining part of the lipid bilayer is chosen close to experimental results (Wedlich-Söldner group, University of Münster). From these simulations we gain insight into structural properties such as of e.g. the order parameter, the RDF or the interdigitation. This allows a deeper understanding of the order of the long-chain spingolipids, their effect on the overall membrane structure and the coupling between the leaflets.

BP 19.3 Wed 10:00 H46

Engineering asymmetric lipid vesicles for protein delivery — •Kevin Jahnke, Chenjing Yang, and David Weitz — Harvard University, Cambridge, USA

The delivery of therapeutics to cells is crucial for the treatment and prevention of diseases. To enhance targeting and protect therapeutics from degradation, they are often encapsulated into drug delivery vehicles like lipid nanoparticles, liposomes and viral vectors. However, there is no universal vehicle for all cargo types including small molecules, nucleic acids and proteins. Here, we present a method for engineering lipid vesicles with asymmetric leaflets and demonstrate their ability to deliver mRNA and proteins to cells (Yang,.., Weitz, Jahnke; biorxiv 2024). We show that leaflet asymmetry modulates the biophysical properties of lipid vesicles, leading to an enhanced vesicle uptake by cells, and an up to 5-fold increased transfection efficiency with mRNA. Additionally, we show that asymmetric vesicles can deliver a variety of proteins, including the gene-editing protein Cas9 and Cas9/sgRNA complexes. By modifying lipid vesicles with polysaccharides (Jahnke et al.; PNAS 2024) or the engineering of lipid-polymer hybrid vesicles, we further achieve the targeted delivery to specific cell types. Our method and findings expand the parameter space for engineering drug delivery vehicles and demonstrate the pivotal role of leaflet asymmetry in determining the biophysical properties of lipid vesicles. Consequently, our work leads to many applications, including the formation of more efficient, universal drug carriers that enable the delivery of proteins to cells.

BP 19.4 Wed 10:15 H46

Vesicle to bicelle decomposition can be correlated with the lipid's main phase transition: a direct evidence using chain-deuterated lipid — •Carina Dargel[1,2], Lara H. Moleiro[2], Aurel Radulescu[3], Tim J. Stank[2], and Thomas Hellweg[2] — [1]University of Münster, Institute of Physical Chemistry, Münster, Germany — [2]University of Bielefeld, Physical and Biophysical Chemistry, Bielefeld, Germany — [3]FZ Jülich, Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany

Mixtures of the phospholipid 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) and the saponin β-aescin form bicelles above a critical saponin concentration. Modification of the membrane's phase state by temperature increase induces a structural growth of the bicelles resulting in membrane-like DMPC-aescin aggregates or mixed small unilamellar vesicles.

The temperature-induced transition is fully reversible, independent of the aescin content. Furthermore, the decomposition of the mixed vesicles back to bicelles shows a prominent hysteresis effect, which is correlated with the main phase transition temperature T_m of the lipid. This correlation was demonstrated for the first time by taking advantage of the shift of the membrane's T_m due to chain-deuteration and thus the use of d54-DMPC by both turbidimetry and small angle neutron scattering (SANS)[1].

[1] Dargel *et al.* (2025), Journal of Colloid and Interface Science, 679, 209-220.

BP 19.5 Wed 10:30 H46

Exploring DNA Linkers for Biomimetic Cell Adhesion of Red Blood Cells — •Sebastian W. Krauss[1], Roger Rubio-Sánchez[1], Bortolo M. Mognetti[2], Lorenzo Di Michele[1], and Pietro Cicuta[3] — [1]CEB, University of Cambridge, UK — [2]ULB, Brussels, Belgium — [3]Department of Physics, University of Cambridge, UK

Ligand-receptor interactions are fundamental to cellular membrane dynamics, influencing a range of processes like cell-cell signaling and viral infections. These interactions govern how adjacent membranes recognize, bind, and respond to one another. To better understand these mechanisms, we developed a biomimetic approach that grants precise control over the strength of interactions between opposing membranes. Our strategy employs short membrane-anchored amphiphilic DNA nanostructures featuring single-stranded 'sticky-ends', which are designed to bind through complementary sequences, providing an adaptive platform for membrane-membrane interactions [Chem. Comm. 57, 12725 (2021)]. We implemented our platform to functionalize red blood cells (RBCs), creating cellular aggregates with programmable morphologies, ranging from doublets to star-like geometries. Additionally, we used DNA-functionalized particles to selectively bind RBCs. By tuning the sequence, we precisely controlled interaction strength, enabling RBCs to progressively envelop beads. Furthermore, we employed optical tweezers to observe the rapid formation of strong bonds in situ [manuscripts in preparation]. This system offers insights into the forces and dynamics of RBC aggregation and their interactions with pathogens, such as Plasmodium species responsible for malaria.

BP 19.6 Wed 10:45 H46

Investigating Endosomal Escape Mechanisms of PEI-DNA Polyplexes with Computer Simulations — •Jonas Lehnen[1], Friederike Schmid[1], and Giovanni Settanni[2] — [1]Physik, Johannes Gutenberg Universität, Mainz — [2]Physik, Ruhr-Universität Bochum

Nucleic-acid-based therapeutics have recently demonstrated their potential thanks to the successful COVID-19 vaccination campaign. They have been already approved or in the latest stages of clinical trials as remedies for a broad range of pathologies, including cancer and genetic diseases. These approaches make use of complex delivery vehicles to take the nucleic acids to the target tissues. The presently used lipid-based nanoparticles still face a relatively low delivery rate and side effects. Polyplexes, formed by the aggregation of cationic polymers with the anionic nucleic acids, may provide a valid alternative. The transfection mechanism for these polyplexes is an ongoing topic of research. We use coarse grained molecular dynamics simulations to investigate contributing factors to the endosomal escape process which

is a crucial limiting step in the transfection process. Our simulations model an endosome containing a polyplex, evaluating key factors such as the surface tension of the endosome caused by osmotic swelling and the interactions between the polyplex and the endosomal membrane, which are key factors in the predominant theories.

BP 19.7 Wed 11:00 H46

Modeling endosomal membrane budding patterns — •Felix Frey and Andela Saric — Institute of Science and Technology Austria, Klosterneuburg, Austria

Lipid membranes define cells and structure their interior. Endosomes, which are organelles that host molecular cargo sorting processes, are enclosed by flexible membranes from which small vesicles continuously pinch off. The reshaping of the endosomal membrane is mediated by filamentous proteins of the ESCRT-III family. Strikingly, in endosomes of flowering plant cells, arrays of concatenated membrane vesicles can form, which are connected either in parallel or in series with the membrane base. Here we combine coarse-grained molecular dynamics simulations and continuum theory with electron tomography to study the budding patterns at plant endosomal membranes [1]. We find that changes in ESCRT-III filament properties, such as curvature and membrane binding energy, determine the formation pathways and shapes of the emerging vesicle networks.

[1] E. Weiner*, E. Berryman*, F. Frey*, A. González Solís* et al., Proc. Natl. Acad. Sci. U.S.A. 121.44 (2024): e2409407121. *Equal contributions.

15 min. break

Invited Talk BP 19.8 Wed 11:30 H46

Rolling vesicles: From confined rotational flows to surface-enabled motion — •Laura R. Arriaga[1], Paula Magrinya[1], Pablo Palacios[1], Pablo Llombart[1], Rafael Delgado-Buscalioni[1], Alfredo Alexander-Katz[2], and Juan L. Aragones[1] — [1]Department of Theoretical Condensed Matter Physics, Condensed Matter Physics Center (IFIMAC) and Instituto Nicolás Cabrera, Universidad Autonoma de Madrid, 28049, Madrid, Spain — [2]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

Friction forces are essential for cell movement, yet they also trigger numerous active cellular responses, complicating their measurement in vivo. In this talk, we will introduce a synthetic model designed to measure friction forces between biomimetic membranes and substrates. The model consists of a vesicle with precisely controlled properties, fabricated via microfluidics, encapsulating a single ferromagnetic particle that is magnetically driven to rotate. The rotation of the particle generates a confined rotational flow, setting the vesicle membrane into motion. By adjusting the magnetic field frequency and vesicle size, the rotation frequency of the vesicle can be finely controlled, resulting in a rolling vesicle that functions as an effective tribological tool. At low frequencies, molecular contact between the membrane and substrate dominates frictional interactions, providing a measurement of the contact friction coefficient. Adjusting membrane fluidity within this model will enable the study of frictional processes in more complex biomimetic systems.

BP 19.9 Wed 12:00 H46

Dynamics of a microswimmer near a deformable boundary — •Sagnik Garai, Ursy Makanga, Akhil Varma, and Christina Kurzthaler — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany

We study the hydrodynamic interactions of swimming microorganisms with nearby deformable boundaries omnipresent in their natural habitats. The boundary, characterized by its surface tension and bending rigidity, is deformed by the disturbance flow produced by the microswimmer and thereby modifies its swimming velocities. Describing the far-field flow of the agent as a combination of a force and torque dipole, we compute small deformations of the boundary. We further use the Lorentz reciprocal theorem to obtain leading-order corrections of its swimming velocities and compute a phase diagram based on the swimmer's initial orientation and the material properties of the deformable boundary. Our results reveal that pushers can both re-orient away from the boundary, leading to overall hydroelastic repulsion, or hover near the boundary, while pullers exhibit enhanced attraction. These findings demonstrate that the complex elasto-hydrodynamic interactions can generate behaviors that are fundamentally different to swimming near planar walls.

BP 19.10 Wed 12:15 H46

Uptake of microgels by membrane wrapping — •Tanwi Debnath[1], Jiarul Midya[1,2], Thorsten Auth[1], and Gerhard Gompper[1] — [1]Theoretical Physics of Living Matter, Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]School of Basic Sciences, IIT Bhubaneswar, 752050, India

The interaction of nano- and microcarriers with lipid-bilayer membranes plays a key role for cellular engulfment and drug delivery [1]. The physico-chemical parameters of the particles that control engulfment are their size, shape, and deformability [2]. Microgels are particularly versatile because their elasticity can be tuned in a wide range by changing the density of crosslinkers. Using a mass-spring model for the microgel and a continuum model for the membrane, we study microgel wrapping at lipid-bilayers. We use the Hertz theory to characterize the microgel's Young's modulus and Poisson's ratio. With the help of triangulated membranes and energy minimization, we determine the interplay of microgel and membrane deformation. We predict wrapping diagrams for microgels with various Young's moduli at membranes with various tensions. A higher microgel deformability increases the stability of partial-wrapped states; there is a transition from oblate at low wrapping fractions to cup-like shape at high wrapping fractions. Our results on this tunable and responsive system will allow the design of the microgels with optimal elastic properties for biomedical applications. [1] S. Dasgupta et al., J. Phys. Condens. Matter **29**, 373003 (2017). [2] J. Midya et al., ACS Nano **17**, 1935 (2023).

BP 19.11 Wed 12:30 H46

Shaping Cellular Interfaces — •Susanne Liese[1], Xueping Zhao[2], Tiemei Lu[3], Marcel Mokbel[4], Sebastian Aland[4], Evan Spruijt[3], Frank Jülicher[5], and Christoph Weber[1] — [1]Universität Augsburg — [2]University of Nottingham Ningbo China — [3]Radboud University, Nijmegen — [4]TU Freiberg — [5]Max Planck Institute for the Physics of Complex Systems

The interaction between liquid droplet-like coacervates and biological membranes is central to cellular organization and drives essential processes including endocytosis, intracellular transport, and signaling. In our research, we uncover the complex dynamics underlying these interactions, demonstrating how non-equilibrium processes, chemical activity, and mechanical deformations dictate the behavior of droplet-membrane systems. We demonstrate that non-equilibrium binding of biomolecular condensates to membranes gives rise to rich physical phenomena, and we also reveal how membrane reshaping contributes to behaviors such as anomalous wetting and deformation-driven uptake. By integrating experiments, theoretical models, and computational simulations, our work provides new insights into the mesoscale physics of cellular systems and reveals the intricate interplay of chemical and mechanical forces at the droplet-membrane interface. This understanding advances both fundamental biology and potential applications in synthetic biology and intracellular delivery.

BP 19.12 Wed 12:45 H46

Biomolecular condensates wetting membranes - dynamical insights from numerical simulations — •Sebastian Aland — HTW Dresden — TU Freiberg

Biological cells use membranes and condensates (liquid-like droplets) to compartmentalize their interior. As every structure within a cell is either enclosed by a membrane or by a liquid interface it is fundamental to understand what happens if these two come into contact. Recent studies suggest that membrane-droplet interactions are involved in various key biological processes. As experimental image resolution is limited at the corresponding length and time scales, numerical methods are essential to shed light on the dynamics of the process. Using a combination of sharp and diffuse interface models, we derive a mathematical model to describe the interplay of a thin elastic membrane with a two-phase fluid. We demonstrate that the wetting interaction by capillary forces leads to a range of fascinating phenomena like droplet wrapping, endocytosis and an inverted cheerios effect.

BP 20: Statistical Physics of Biological Systems I (joint session BP/DY)

Time: Wednesday 15:00–18:00 Location: H44

BP 20.1 Wed 15:00 H44

Separating bio-condensates with surfactant-like proteins — Jannik Kindermann and •Tyler Harmon — Leibniz Institute for Polymer Research, Dresden, Germany

Biocondensates are prevalent in cells as individual compartments that separate material and reactions in space. Many condensates share similar components and/or chemical interactions that drive their formation. This would suggest that the condensate:condensate interface would have a very low surface tension compared to the condensate:solvent interfaces. Supported by in vitro results, this leads to condensate-inside-condensate or dumbbell-like architectures which minimize the condensate:solvent interfaces. However, in vitro, condensates are most often isolated in space from each other. This could play important roles such as limiting the direct flow of material from one condensate to another. The mechanism in cells that separates droplets in space is unknown.

We show using simulations and theory that proteins or other biopolymers that have surfactant like molecular architectures can separate condensates in space. We show how robust this mechanism can be with respect to condensate specificity and the expression levels of surfactant-like molecules in cells.

BP 20.2 Wed 15:15 H44

Phase separation in membranes and compartments with binding reactions — •Riccardo Rossetto, Gerrit Wellecke, and David Zwicker — Max Planck Institute for Dynamics and Self-Organization

Biological cells exhibit a hierarchical spatial organization, where various compartments and membranes harbor condensates that form by phase separation. Cells can control the emergence of these condensates by affecting the physical interactions of the involved biomolecules, thus also tuning the binding affinity to the compartments. We describe this situation with a thermodynamically-consistent kinetic model considering passive and active binding reactions to elucidate their role in controlling the occurrence and timescales of phase separation in compartments. On the one hand, binding reactions can lead to the emergence of new equilibrium phenomena, such as re-entrant phase transitions and multistability. On the other hand, they can also affect the kinetics of phase separation. As a particular example, we consider protein droplets in cellular membranes when proteins can also unbind to the cellular bulk. For fast bulk diffusion, this leads to effective nonlocal transport, which fundamentally affects droplet dynamics. For instance, the seminal Lifshitz-Slyozov coarsening can be abolished. Furthermore, active binding reactions can both accelerate or fully suppress coarsening, leading to protein patterns on the membrane. The general conclusions from our model unveil fundamental mechanisms of phase separation in membranes and compartments, and will help us explain more biological observations in the future.

BP 20.3 Wed 15:30 H44

Reconciling conflicting selection pressures in the plant collaborative non-self recognition self-incompatibility system — Amit Jangid[1], Keren Erez[1], Ohad-Noy Feldheim[2], and •Tamar Friedlander[1] — [1]Faculty of Agriculture, food and environment, The Hebrew University of Jerusalem, Rehovot, Israel — [2]Einstein Institute for Mathematics, The Hebrew University of Jerusalem, Jerusalem, Israel

Complex biological systems should often reconcile conflicting selection pressures. Specifically, in systems relying on molecular recognition, molecules should recognize particular partners, but avoid others. Here we study how such selection pressures shape the evolution of the self-incompatibility system in plants. This system inhibits self-fertilization using specific molecular recognition between proteins, expressed in the plant female and male reproductive organs. We study the impact of these opposing selection pressures on the amino acid frequencies in these proteins' recognition domain. We construct a theoretical framework enabling promiscuous recognition between proteins and multiple partners each, as found empirically, and employ stochastic simulations. We find asymmetric responses to selection affecting mostly the female, but not the male protein composition. Using large deviations theory, we well-approximate the simulated frequencies and find agreement with genomic data. Our work offers a general theoretical framework to study the impact of multiple selection pressures, applicable to additional biological systems.

BP 20.4 Wed 15:45 H44

Learning the Equilibrium Free Energy from Non-Equilibrium Steady States with Denoising Diffusion Models — •Daniel Nagel and Tristan Bereau — Institute for Theoretical Physics, Heidelberg University, 69120 Heidelberg, Germany

Estimating accurate free energy profiles is crucial for predicting the behavior of complex molecular systems. While biased molecular dynamics simulations enhance the sampling of rare events, extracting reliable free energy landscapes from these simulations remains challenging. On the other hand, stochastic thermodynamics, i.e. the concept of entropy production, provides valuable insights into the dynamics of complex systems in non-equilibrium states. However, its computational complexity, due to dependence on time-dependent probability distributions, limits its application to smaller systems.

This work presents a novel approach that combines stochastic thermodynamics with the established machine learning technique of denoising diffusion models to efficiently estimate free energy profiles from biased non-equilibrium steady states. By linking the diffusion and simulation times, we show that the training objective, known as the score, can be decomposed into a non-trivial conservative contribution from the equilibrium potential and a trivial non-conservative part determined by external driving forces. To showcase the effectiveness of our approach and its ability to learn equilibrium free energy profiles, we apply it to a driven toy model and a Martini force field molecular dynamics simulation of a small molecule biased through a lipid bilayer.

BP 20.5 Wed 16:00 H44

Multiple Pareto-optimal solutions of the dissipation-adaptation trade-off — •Jorge Tabanera-Bravo and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen

Adaptation refers to the ability to recover and maintain "normal" function upon perturbations of internal or external conditions and is essential for sustaining life. Biological adaptation mechanisms are dissipative, i.e. they require a supply of energy such as the coupling to the hydrolysis of ATP. Via evolution the underlying biochemical machinery of living organisms evolved into highly optimized states. However, in the case of adaptation processes two quantities are optimized simultaneously, the adaptation speed or accuracy and the thermodynamic cost. In such cases one typically faces a trade-off, where improving one quantity implies worsening the other. The solution is no longer unique but rather a Pareto set—the set of all physically attainable protocols along which no quantity can be improved without worsening another. We investigate Pareto fronts in adaptation-dissipation trade-offs for a cellular thermostat and a minimal ATP-driven receptor-ligand reaction network. We find convex sections of Pareto fronts to be interrupted by concave regions, implying the existence of distinct optimization mechanisms. We discuss the implications of such "compromise-optimal" solutions and argue that they may endow biological systems with a superior flexibility to evolve, resist, and adapt to different nvironments.

15 min. break

Invited Talk BP 20.6 Wed 16:30 H44

Centrosome positioning in cell migration and immune response — •Heiko Rieger — Department of Physics and Center for Biophysics, Saarland University, Saarbrücken, Germany

Leukocytes are the key players of the immune system in eliminating pathogen-infected or tumorigenic cells. During these processes centrosome positioning plays a crucial role for establishing cell polarization and directed migration, targeted secretion of vesicles for T cell activation and cellular cytotoxicity as well as the maintenance of cell integrity. Here, we give an overview over microtubule organization and dynamics during immune processes and present models for centrosome repositioning during the formation of the immunological synapse and during cell migration. We focus particularly on actin-myosin crosstalk, which is involved in regulating the polarity and morphology of migrating cells and encompasses mechanical interactions, mediated by crosslinkers and molecular motors, as well as cytoskeletal

regulators. Based on recent experimental results we develop a computational whole-cell model involving dynamical microtubules that interact not only mechanically but also via signaling with an active cell boundary. A rich self-organized dynamical behavior emerges, comprising varying positions of the microtubule organizing center relative to the nucleus in the migration direction, varying migration characteristics and cell shapes, and complex migratory behavior in obstacle parks and microfluidic setups. Specific dependencies of these behaviors from parameters like the average microtubule length or the cell-boundary stiffness are predicted and compared with experimental observations.

BP 20.7 Wed 17:00 H44

Modelling neuron growth dynamics and role of extra-cellular matrix — •Pritha Dolai, Federica Furlanetto, Sven Falk, Marisa Karow, and Vasily Zaburdaev — Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg, Erlangen

Biological tissues are composed of cells embedded in extracellular matrix (ECM) and extracellular fluid. We study the role of cell-matrix interactions in the context of brain tissues and the mechanism of neuron growth through this matrix. We consider two modes for the neurite growth: linear growth by tip extension and growth by the traction force at the tip of the neurite with the ECM. In the second mechanism, growth happens solely due to the interaction of the growing appendages with the particles modeling the matrix. With an agent based model we recapitulate experimentally observed neuron growth patterns in healthy neurons and neurons with mutations corresponding to a disease state performed in organoid models. In experiments, neuron growth is quantified by the dynamics of the growing tips. Additionally we compare further growth characteristics such as track length and velocity of the tip, tortuosity, and angular correlation of growth direction. Our model provides mechanistic description of the neurite growth and can be useful in describing neuronal network formation during early development.

BP 20.8 Wed 17:15 H44

Cellular morphodynamics as quantifiers for functional states of resident tissue macrophages in vivo — •Miriam Schnitzerlein[1,2], Eric Greto[3,4], Anja Wegner[3,4], Anna Möller[3,4], Oliver Aust[3,4], Oumaima Ben Brahim[3,4], Stefan Uderhardt[3,4], and Vasily Zaburdaev[1,2] — [1]Department of Biology, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen — [3]Department of Medicine 3 - Rheumatology and Immunology, FAU und Universitätsklinikum Erlangen — [4]Deutsches Zentrum für Immuntherapie, FAU

Resident tissue macrophages (RTMs) perform essential tasks such as clearing cellular debris to ensure tissue homeostasis. Such actions are accompanied by morphological changes in cell shape which reflect their functional states. Until now, RTMs were mostly studied *in vitro*, even though their dynamic behaviour *in vivo* is fundamentally different.

We employed a high-resolution, intravital imaging protocol to generate dynamic data of *in vivo* peritoneal RTMs of mice. Next we built a custom image processing pipeline to assess RTM morphodynamics via a set of human-interpretable cell shape and size features. Those features could quantitatively and also qualitatively differentiate between cells in different activation states. Furthermore, we showed that unperturbed RTMs exhibit a wide range of morphodynamical phenotypes, constituting a naive morphospace of behavioural motifs. Analysing cells challenged by chemical stimulations or due to aging gave us insights into how RTMs respond and adapt to inflammatory stimuli.

BP 20.9 Wed 17:30 H44

Slimming down through frustration — •Martin Lenz — Université Paris-Saclay, CNRS, LPTMS, 91405, Orsay, France — PMMH, CNRS, ESPCI Paris, PSL University, Sorbonne Université, Université Paris-Cité, F-75005, Paris, France

In many disease, proteins aggregate into fibers. Why? One could think of molecular reasons, but here we try something more general. We propose that when particles with complex shapes aggregate, geometrical frustration builds up and fibers generically appear. Such a rule could be very useful in designing artificial self-assembling systems.

BP 20.10 Wed 17:45 H44

RNA fitness prediction with sparse physics based models - A way to explore the sequence space — •Christian Faber[1], Francesco Calvanese[2], Alexander Schug[1], and Martin Weigt[3] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Sorbonne-Université, Paris, France — [3]CNRS, Paris, France

The field of medicine uses macromolecules as a means of therapeutic intervention. Consequently, the functional attributes of these novel molecules are assuming greater significance. To complement the wet-lab experiments, we have devised a series of statistical physics based models that are capable of predicting the fitness of RNA molecules based on one- and two-point mutation scans. The experimental data were employed as training data to fit models of increasing complexity, commencing with an additive model and concluding with a model that accounts for global and local epistasis. The models were validated using fitness data from scans with higher order mutations of the wild-type. In contrast to conventional AI algorithms, the parameters of our models were designed for direct interpretation. In examining more distant sequences, we can distinguish the corresponding RNA family from random sequences with a high degree of accuracy. Moreover, the models facilitate interpretations of evolutionary processes and the significance of epistatic terms. Our model can be used to create a fitness landscape far beyond the experimental sequence space, thus identifying promising RNA molecules. Furthermore, the extension to the entire sequence space can be used as a blueprint for other molecules, providing a novel avenue for questions in biomolecular design.

BP 21: Networks, From Topology to Dynamics (joint session SOE/BP/DY)

Time: Wednesday 15:00–17:30 Location: H45

BP 21.1 Wed 15:00 H45

Self-organized transport in noisy dynamic networks — •Frederic Folz[1], Joshua Rainer Ganz[1], Kurt Mehlhorn[2], and Giovanna Morigi[1] — [1]Theoretische Physik, Universität des Saarlandes, 66123 Saarbrücken, Germany — [2]Algorithms and Complexity Group, Max-Planck-Institut für Informatik, Saarland Informatics Campus, 66123 Saarbrücken, Germany

We present a numerical study of multicommodity transport in a noisy, nonlinear network. The nonlinearity determines the dynamics of the edge capacities, which can be amplified or suppressed depending on the local current flowing across an edge. We consider network self-organization for three different nonlinear functions: For all three we identify parameter regimes where noise leads to self-organization into more robust topologies, that are not found by the sole noiseless dynamics. Moreover, the interplay between noise and specific functional behavior of the nonlinearity gives rise to different features, such as (i) continuous or discontinuous responses to the demand strength and (ii) either single or multistable solutions. Our study shows the crucial role of the activation function on noise-assisted phenomena.

BP 21.2 Wed 15:15 H45

Critical properties of Heider balance on multiplex networks — •Krishnadas Mohandas, Krzysztof Suchecki, and Janusz Hołyst — Faculty of Physics, Warsaw University of Technology, Koszykowa 75, PL-00-662 Warsaw, Poland

Heider's structural balance theory has proven invaluable in comprehending the dynamics of social groups characterized by both friendly and hostile relationships. Extending this understanding to multiplex networks, we investigate Heider balance dynamics in systems where agents exhibit correlated relations across multiple layers. In our model, intralayer interactions adhere to Heider dynamics, while interlayer correlations are governed by Ising interactions, using heat bath dynamics for link signs. This framework reveals a multifaceted equilibrium landscape, with distinct phases coexisting across layers. Starting from a paradise state with positive links in all layers, increasing temperature induces a discontinuous transition to disorder, similar to single-layer scenarios but with a higher critical temperature, as verified through extended mean-field analysis and agent-based simulations.

We extend this analysis to Erdös-Rényi random graphs in noisy environments. We predict a first-order transition with a critical temperature scaling as p^2 for monolayers and follow a more complex behav-

ior for bilayers. To replicate dynamics observed in complete graphs, intralayer Heider interaction strengths must scale as p^{-2}, while interlayer interaction strengths scale as p^{-1} in random graphs. Numerical simulations confirm these analytical predictions for dense graphs.

BP 21.3 Wed 15:30 H45

Functional Motifs in Food Webs and Networks — •Melanie Habermann[1,2,3], Ashkaan Fahimipour[4], Justin Yeakel[5,6], and Thilo Gross[1,2,3] — [1]Helmholtz Institute for Functional Marine Biodiversity (HIFMB), Oldenburg, GER — [2]Alfred-Wegener Institute (AWI), Helmholtz Center for Polar and Marine Research, Bremerhaven, GER — [3]Carl-von-Ossietzky University, Institute for Chemistry and Biology of the Marine Environment (ICBM), Oldenburg, GER — [4]Florida Atlantic University, Boca Raton, FL, USA — [5]University of California Merced, Merced, CA, USA — [6]The Santa Fe Institute, Santa Fe, NM, USA

It is interesting to ask when the presence of a small subgraph in a complex network is sufficient to impose constraints on system dynamics that are independent of the broader network structure. We refer to these subgraphs as functional motifs. A classic example can be found in ecology with the competitive exclusion motif in food webs, where two species compete for the same resource without regulation. The presence of this motif precludes any stable equilibrium for the entire system. However, examples of other motifs with similarly definitive implications for system stability are rare. But our usual notion of asymptotic stability is just one among many different concepts of stability. Another one, reactivity, captures a system's immediate response to small perturbations. In this talk, we explain why functional stability motifs are rare and show that every subgraph is a functional reactivity motif. This highlights reactivity as a promising concept for exploring a vast range of networked phenomena.

BP 21.4 Wed 15:45 H45

Infecting Apex Predators Could Lead to Their Extinction — •Fakhteh Ghanbarnejad[1] and Hooman Saveh[2] — [1]SRH University of Applied Sciences, Leipzig, Germany — [2]Sharif University of Technology, Tehran, Iran

Food webs have been extensively studied from both ecological and mathematical aspects. However, most of the models studied in this area do not capture the effects of infectious diseases simultaneously. Recently, the idea of including an infectious disease in a food web model has been investigated. We study and simulate a small food chain consisting of only prey, predators, and apex predators governed by the generalized Lotka-Volterra equations and we implement the Susceptible-Infected-Recovered (SIR) model on only one of the species at a time in the food chain. To study the effects of an infectious disease on the food chain, we introduce a new parameter that increases predation rate by a factor of w and decreases hunting rate by a factor of $1/w$ for infected species. When the infectious disease is in our predators we observe that predators do not extinct under any set of parameters, however, an oscillation in its population size occurs under some circumstances which we do not observe in ordinary SIR or the generalized Lotka-Volterra equations alone. When an infectious disease is present in apex predators, oscillations in the population size do not happen; but if the set of parameters is in a specific range the apex predators may extinct. Furthermore, the chance of survival of the community, known as community persistence, increases for the predators and decreases for the apex predators.

15 min. break

BP 21.5 Wed 16:15 H45

Behavioral Heterogeneity in Disease Spread: Contrasting Effects of Prevention Strategies and Social Mixing — •Fabio Sartori[1,2] and Michael Maes[1] — [1]Chair of Sociology and Computational Social Science, Karlsruhe Institute of Technology, Karlsruhe — [2]Max Planck Institute for Dynamics and Self Organisation, Göttingen, Germany

Despite mounting evidence of behavioral heterogeneity in response to disease threats, the majority of epidemiological models assume uniform behavior across populations for mathematical tractability. We analyze three distinct mechanisms of behavioral response to disease threat: susceptibility reduction (e.g., mask-wearing), active testing, and vaccination propensity. Through extensive numerical analysis, we demonstrate that the impact of behavioral heterogeneity strongly depends on the specific mechanism involved. While heterogeneous susceptibility-reducing behaviors generally decrease disease spread, heterogeneity in testing rates and vaccination propensity typically amplifies epidemic severity. Furthermore, we show that non-homogeneous mixing patterns, particularly when correlated with behavioral traits, exacerbate disease spread across all three mechanisms. These findings reveal fundamental principles about the interplay between behavioral heterogeneity and epidemic dynamics, challenging the conventional homogeneous assumption and providing important implications for public health interventions and policy design.

BP 21.6 Wed 16:30 H45

Modelling retweet cascades using multivariate Hawkes processes on sparse networks — Alexander Kreiss[1] and •Eckehard Olbrich[2] — [1]Leipzig University, Germany — [2]Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany

We apply a model that considers vertices in a network who are able to cast events, e.g. users of the online social media platform Twitter. Furthermore, there is a directed edge from vertex A to vertex B if A takes note of the events cast by B and changes its own behavior accordingly. More precisely, the model assumes that the activity of B increases the activity of A and likewise its other neighbors. This is called peer effects. However, there might also be other information, which also influences the activity of the vertices, e.g. the time of the day for social media posts. This is called global effects. We use a Hawkes model that incorporates, both, peer and global effects. This allows for the estimation of the network, that is, the influence structure while controlling for network effects or the estimation of the global effects while controlling for peer effects. The estimation is based on a LASSO strategy, which respects sparsity in the network. We apply this model to retweets on Twitter in order to reconstruct potential retweet cascades and identify accounts that are influential in sharing information.

BP 21.7 Wed 16:45 H45

Influence, Incidence, Imitators and Individualists: Comparing social influence models of protective behavior in an epidemic — •Andreas Reitenbach — Karlsruhe Institute of Technology, Karlsruhe, Germany

To manage a pandemic, it is critical that citizens voluntarily engage in protective behavior (e.g. masking or vaccinating). Voluntary behavior is subject to complex dynamics of social influence, however. While various models couple social influence dynamics with disease spreading, assumptions about how individuals influence each other differ markedly. Models assuming herding implement that agents imitate their peers. On the contrary, rational agents (individualists) engage in protective behavior when their peers are not and vice versa, potentially free-riding on others' contributions to herd immunity.

Here, I study whether and why these competing behavior models translate into different disease dynamics. Following a recent call to abstract from psychological mechanisms underlying social influence, I translate the behavior theories into influence-response functions.

I find that individualists self-coordinate on a moderate level of protection and experience long-lasting but flat incidence curves. Herding, in contrast can result in rapid cycling through waves of high incidence and strong collective efforts to mitigate. Whether herders or individualists navigate an epidemic better can depend on the population's hospital capacity and disease parameters.

BP 21.8 Wed 17:00 H45

Formalism and Physical Principles of Human Mobility and Routine — •Marlli Zambrano[1], Ashish Thampi[2], Alejandra Rincon[2], Andrzej Jarynowski[1], Steven Schulz[2], and Vitaly Belik[1] — [1]Freie Universität Berlin, Germany — [2]Machine Learning Unit, NET CHECK GmbH, Berlin, Germany

The physical principles underlying human mobility have been extensively studied in recent years, enabled by the availability of large-scale mobile phone data. While significant progress has been made in understanding general mobility patterns, capturing the dynamics of individual trajectories, specifically how mobility varies from person to person and day to day, remains challenging due to the need for highly detailed and persistent data. This study addresses this challenge by examining sequences of individual daily mobility motifs, as defined by Schneider et al., from a stochastic process perspective. The analysis uses a persistent mobile phone user panel in Berlin, with high-frequency GPS data collected over four years. Twenty motifs were identified, covering 96% of all observations. The extent of inter- and intra individual variability is explored, focusing on how motifs change within individ-

uals over time and differ between individuals in various contexts (e.g., weekends, seasons). Additionally, sequences of motifs are modeled as a stochastic process, and properties such as transition probabilities are analyzed. These findings provide deeper insights into the variability and structure of human mobility, contributing to a better understanding of individual mobility dynamics.

BP 21.9 Wed 17:15 H45

The world air transportation network: import risk of diseases, pandemic potentials and passenger routes — •Pascal Klamser[1,2], Adrian Zachariae[1,2], Benjamin Maier[3], Olga Baranov[4], and Dirk Brockmann[1,2] — [1]Technische Universität Dresden, Dresden, Germany — [2]Robert Koch-Institute, Berlin, Germany — [3]University of Copenhagen, Copenhagen, Denmark — [4]LMU München, München, Germany

Disease propagation between countries strongly depends on their effective distance, a measure derived from the world air transportation network. It reduces the complex spreading patterns of a pandemic to a wave-like propagation from the outbreak country, establishing a linear relationship to the arrival time of the unmitigated spread of a disease. However, in the early stages of an outbreak, what concerns decision-makers in countries is understanding the relative risk of active cases arriving in their country*essentially, the likelihood that an active case boarding an airplane at the outbreak location will reach them. While there are data-fitted models available to estimate these risks, accurate mechanistic, parameter-free models are still lacking.

We (i) introduce the "import risk" model, which defines import probabilities using the effective-distance framework, (ii) show its application to estimate the pandemic potential of emerging variants of COVID-19 and (iii) show that the effective distance shortest path tree, on which the "import risk" model is based on, is an extremely accurate representation of true passenger routes.

BP 22: Bioimaging

Time: Wednesday 15:00–17:45 Location: H46

Invited Talk BP 22.1 Wed 15:00 H46

From DNA Nanotechnology to biomedical insight: Towards single-molecule spatial omics — •Ralf Jungmann — LMU and MPI of Biochemistry, Munich, Germany

Super-resolution fluorescence microscopy is a powerful tool for biophysical and biological research. The transient binding of short fluorescently labeled oligonucleotides (DNA-PAINT) can be leveraged for easy-to-implement multiplexed super-resolution imaging that achieves molecular-scale resolution across large fields of view. This seminar will introduce recent technical advancements in DNA-PAINT including approaches that achieve sub-10-nm spatial resolution and spectrally unlimited multiplexing in whole cells followed by recent developments in novel protein labeling probes that have the potential to facilitate DNA-barcoded labeling of much of the proteome within intact cellular environments. Applications of these new approaches will be discussed in cell surface receptor imaging and neuroscience. Visualization and quantification of cell surface receptors at thus far elusive spatial resolutions and levels of multiplexing yield fundamental insights into the molecular architecture of surface receptor interactions thus enabling the future development of more refined *pattern*-based therapeutics. A key approach in implementing these methods has been to leverage standard off-the-shelf fluorescence microscopy hardware as a tool for spatial omics, thus democratizing the ability to visualize most biomolecules and probe their network-wide interactions in single cells, tissues, and beyond with single-molecule-based "Localizomics".

BP 22.2 Wed 15:30 H46

3D Single-Nanoparticle Tracking with Fluorescence Lifetime Imaging for Investigating Lipid Nanoparticles Endosomal Pathways — •Thomas Kellerer[1,2], Judith A. Müller[2], Tanja Grawert[1], Lukas Moser[1], Joachim O. Rädler[2], and Thomas Hellerer[1] — [1]Multiphoton Imaging Lab, Munich University of Applied Sciences, 80335 Munich, Germany — [2]Faculty of Physics and Center for NanoScience, Ludwig Maximilians-University, 80539 Munich, Germany

Lipid nanoparticles (LNPs) are vital for delivering mRNA in drug delivery systems, but the kinetics and intracellular pathways of their cargo release remain often unclear. To address this, we developed a microscopy technique to track single nanoparticles in 3D over extended periods. This approach integrates a lock-in amplifier for simultaneous image based 3D tracking and fluorescence lifetime measurement, enabling analysis of the microenvironment, such as pH changes. Achieving a frame rate of 7.6 fps at 1024x1024 resolution and lifetimes measured within 102 ns, our method provides novel insights into LNP dynamics and endosomal acidification in live cells. This technique was applied to study the acidification kinetics of endosomes during transfection. By measuring pH changes in real time, we provided insights into the intracellular behavior of LNPs and their role in mRNA delivery. This approach establishes a new standard for tracking nanoparticles and analyzing their microenvironments with high spatial and temporal resolution.

BP 22.3 Wed 15:45 H46

The dynamics of binding and uptake of SARS-CoV-2 virus-like particles investigated by ROCS and fluorescence microscopy — •Alexander Rohrbach and Dominik Huber — Lab for Bio- and Nano-Photonics, University of Freiburg, Germany

Viruses such as coronavirus SARS-CoV-2 are challenging to observe during interactions with sales in life-cell imaging to their small size and remarkable speed. Techniques like fluorescence microscopy often struggle to visualize these interactions, especially due to their susceptibility to bleaching and the difficulty to label different structures without altering their function.

In our research we use 200 Hz Rotating Coherent Scattering (ROCS) microscopy in order to visualize the diffusion of 100 nm sized virus-mimicking particles (VLPs) and their interactions with macro*phages or epithelial cells. ROCS is a label-free imaging technique at 160 nm resolution, using coherent backscattering of a rotating laser. By tracking VLPs with ROCS and with fluorescence, we are able to analyze their fluctuations and thereby the dynamics of diffusing VLPs close to A549 lung epithelial cells. Using spatiotemporal and spectral analysis methods, we can investigate for the first time diffusion, binding and uptake events of single VLPs at the cell periphery.

BP 22.4 Wed 16:00 H46

Visualising immune cell interactions in lymph nodes — •Anna Schepers[1], Joannah Fergusson[1], Helena Coker[1], Robert Kochl[2], and Marco Fritzsche[1] — [1]Kennedy Institute of Rheumatology, Oxford, UK — [2]King's College London, UK

The inherently multiscale immune response is regulated by diverse cell interactions, relying on cues from tissues down to single cells and subcellular structures. The intricate dynamics of the immune system present challenges for the observation of the immune response. A technological advance has been achieved with the introduction of lattice light sheet microscopy (LLSM), allowing fast and gentle imaging of live samples while achieving subcellular resolution. By complementing LLSM-based volumetric imaging with advanced sample handling of *ex vivo* tissue samples and perfusion imaging chambers, we provide a system that preserves critical physiological complexity. The perfusion system ensures oxygen and nutrient supply to maintain and sample viability while, at the same time, enabling imaging of the perfused samples. We show that in our setup, we can follow single cells and their interactions in volumes several cell layers deep in living samples within their environment, providing nuanced insights into the immune response.

15 min. break

BP 22.5 Wed 16:30 H46

Platelet biomechanics in biochemical confinement — •Vincent Gidlund, Aylin Balmes, and Tilman Schäffer — Institute of Applied Physics, University of Tübingen, Tübingen, Germany

Platelets, as part of the human blood, play a critical role in wound healing, hemostasis, and thrombotic diseases. When platelets accumulate and form plugs during wound healing, they can experience confining microenvironments. For a deeper understanding of platelet

biomechanics, it is important to investigate the effects of a confining microenvironment on platelets. It is known that platelets can adapt to line-shaped microenvironments, but the mechanical properties of platelets subjected to two-dimensional confining microenvironments remain unexplored. We use microcontact printing of fibrinogen patterns of different shapes (circles, triangles) and areas to create a biochemically confining microenvironment for platelets. We then apply epifluorescence microscopy and scanning ion conductance microscopy (SICM) to measure F-actin distribution, topography, and stiffness of platelets confined to these shapes. We found that platelets adapt their morphology to match the shape of the underlying fibrinogen pattern. They show a redistribution of F-actin towards the periphery, as has been observed in other cell types. Additionally, a reduced shape area leads to decreased platelet stiffness.

BP 22.6 Wed 16:45 H46

Near infrared fluorescent silicate nanosheets for Bioimaging — •Bjoern F. Hill and Sebastian Kruss — Physical Chemistry II, Ruhr-University Bochum, Bochu, Germany

Fluorophores emitting in the near-infrared (NIR) are highly advantageous in photonics and biosensing due to reduced light scattering, low phototoxicity, and minimal autofluorescence in this spectral region.

Egyptian Blue (CaCuSi4O10) combines properties that make it a promising material for bioimaging and -photonics: It exhibits bright and stable NIR fluorescence (λ_em=935 nm), its layered structure enables exfoliation into 2D nanosheets (EB-NS), additionally it features a high quantum yield, proven biocompatibility and low production costs.

We present a surfactant-assisted exfoliation route to produce monodisperse EB-NS, tailored to nm-scale diameters, with thicknesses as low as single monolayers, while retaining their NIR fluorescence [1].

Addidionally, we demonstrate the integration of EB-NS with single-walled carbon nanotubes (SWCNTs) to create a ratiometric fluorescence sensor for dopamine. This sensor achieves robust, non-invasive imaging of neurotransmitter release from live cells, while the remarkable stability of the EB-NS fluorescence compensates for environmental fluctuations and enhances measurement reliability [2].

In summary, EB-NS represent a novel, accessible, and highly stable NIR fluorescent nanomaterial with broad applications in bioimaging and -photonics.

[1] B. Hill, et. al., RSC Adv., 2023,13, 20916-20925
[2] B. Hill, J. Mohr, et.al., Nanoscale, 2024,16, 18534-18544

BP 22.7 Wed 17:00 H46

Lysosomal activity in response to incubation of pristine and functionalized carbon nanodots — •Carla Sprengel[1], Céline David[2], Lena Berning[2], Cathrin Nollmann[1], Björn Stork[2], and Thomas Heinzel[1] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Institute of Molecular Medicine I, Medical Faculty and University Hospital Düsseldorf, Heinrich Heine University, Düsseldorf, Germany

Fluorescent carbon nanodots (CNDs) have emerged as promising carriers for drug delivery systems due to their high biocompatibility and functionalizability. We could not find an influence of CNDs on cellular lysosomal functions, as characterized via the cathepsin B and L activity and autophagic markers p62 and LC3B-II, even under high CND concentrations. Functionalization of CNDs with branched polyethylenimin (bPEI) as a model drug conjugate leads to a greater accumulation of bPEI-CND compounds within lysosomes compared to native CNDs. Here, changes in the lysosomal size and function can be explained exclusively by bPEI. This leads us to conclude that CNDs are highly efficient and inert carriers for delivering functional molecules into lysosomes as target while minimizing lysosomal escape and therefore preventing unintended side effects on other cell organelles.

BP 22.8 Wed 17:15 H46

Grating Based X-ray Phase Contrast CT with Laboratory Setups — •Luka Gaetani[1,2], Josef Scholz[1,2], Lorenz Birnbacher[2,3], and Julia Herzen[1,2] — [1]Research Group Biomedical Imaging Physics, Department of Physics, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany — [2]Chair of Biomedical Physics — [3]Institute for Diagnostic and Interventional Radiology, TUM Klinikum rechts der Isar, 81675 München, Germany

Grating-based X-ray Phase Contrast Computed Tomography (CT) represents a significant advancement in imaging, offering enhanced sensitivity to soft tissues and low-density materials by capturing phase information complementary to absorption contrast. This technique utilizes a series of optical gratings to measure phase shifts introduced by the sample, enabling the reconstruction of high-resolution phase contrast images. Laboratory-based implementations of this method, facilitated by compact X-ray sources and precise grating alignment, have extended its accessibility and applicability to diverse fields. However, optimizing these setups necessitates addressing challenges such as coherence management, efficient data acquisition, and advanced reconstruction algorithms to maximize their performance in non-synchrotron environments. This presentation will demonstrate how a grating-based interferometer enables the quantitative determination of electron density, a physical property of the sample, by accurately correlating the sample's influence on the gray values in the recorded X-ray images.

BP 22.9 Wed 17:30 H46

Nanomaterials: A Versatile Sensitizer for Enhanced Singlet Molecular Oxygen Generation — •Zahid Ullah Khan[1], Latif Ullah Khan[1,2], Hermi Felinto Brito[1], and Paolo Di Mascio[1] — [1]Institute of Chemistry, University of São Paulo (USP), 05508-000, São Paulo-SP, Brazil — [2]Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME) P.O. Box 7, Allan 19252, Jordan

Singlet molecular oxygen (1O2) plays a crucial role in various fields, including optoelectronics, photooxygenation reactions, and biomedical therapies, particularly as a major contributor to the success of photodynamic therapy (PDT). Since direct excitation of oxygen from the triplet ground state (3O2) to the singlet-excited state is spin-forbidden, thus, making the design of heterogeneous sensitizers crucial for efficient 1O2 production. For this purpose, nanomaterials, such as quantum dots (QDs) and rare earth fluoride nanoparticles (NPs), have emerged as versatile sensitizers for 1O2 generation, either individually or in combination with other inorganic or organic materials. Hence, conjoining the photophysical properties of QDs and rare earth NPs with other materials, e.g., coupling/combining with other inorganic materials, doping with the transition metal ions or lanthanide ions, and conjugation with a molecular sensitizer provide the opportunity to achieve high-efficiency quantum yields of 1O2 which is not possible with either component separately. Hence, the current work focuses the development of semiconductor QDs and rare earth-based nanosensitizer for efficient production of 1O2.

BP 23: Poster Focus Session Chemical Imaging for the Elucidation of Molecular Structure (joint session O/BP)

Time: Wednesday 18:00–20:00 Location: P2

BP 23.1 Wed 18:00 P2

Imaging of structure, conformation, and assembly of biological molecules by scanning probe microscopy (SPM) — •Joshua Holloway, Márkó Grabarics, Banjamin Mallada, Alejandro Lynch Gonzalez, Lukas Eriksson, and Stephan Rauschenbach — University of Oxford, Oxford, UK

Direct imaging of (bio)molecules by scanning probe microscopy (SPM) is a powerful approach for molecular structure elucidation. Sample preparation presents a challenge: an analyte must be taken into the gas phase, and intactly deposited on the sample surface. Because many biological molecules we wish to study are incompatible with sublimation, we employ electrospray ion beam deposition (ES-IBD). A novel, custom-built deposition stage extending a commercial mass spectrometer (Thermo Fisher Q Exactive UHMR) allows for mass-filtered, soft-landed deposition onto atomically flat metal crystals for high-performance SPM imaging.

Here we present the workflow of mass spectrometry, selection, deposition, and imaging for several examples of biological molecules. In particular we explore the imaging of molecular assemblies of biomolecules with large and small ligands, formed in the gas-phase and/or on the surface.

BP 24: Members' Assembly

Time: Wednesday 18:15–19:15 Location: H46

All members of the Biological Physics Division are invited to participate.

BP 25: Cell Mechanics II

Time: Thursday 9:30–13:00 Location: H44

Invited Talk BP 25.1 Thu 9:30 H44

Oncogenic signaling and stiffness sensing — •Johanna Ivaska — University of Turku

Tissue homeostasis is dependent on the spatially controlled localization of specific cell types and the correct composition of the extracellular stroma. Integrin-mediated adhesions, in conjunction with the actin cytoskeleton and signaling by receptor tyrosine kinases, regulate cell fate and identity and allow cells to migrate and invade the surrounding extra-cellular matrix (ECM). We have previously uncovered key differences between normal and cancer-associated stroma, whereby the mechanical and architectural features of normal stroma inhibit tumour growth and may epigenetically reprogram aggressive breast cancer cells towards a more benign phenotype. Recently, we turned our attention to other putative crosstalk mechanisms between cancer cells and the tumor microenvironment as well as tumor cell interactions with distinct tissue borders during systemic dissemination in the body. I will describe different control mechanisms guiding cancer cell invasion across physiological borders and their relevance to cancer progression and metastasis.

BP 25.2 Thu 10:00 H44

Perfect stabilization of biomolecular adhesions under load — •Anton Francis Burnet[1,2] and Benedikt Sabass[1,2] — [1]Department of Veterinary Sciences, Ludwig-Maximilians-Universität München, 80752 Munich, Germany — [2]Faculty of Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, 80752 Munich, Germany

Cell focal adhesions are complex molecular assemblies that demonstrate the remarkable capability to adapt to mechanical load by changing their size. Drawing from the molecular mechanisms believed to drive this behavior, we present a minimal adhesion model for mechanically induced aggregation of adhesion molecules. If the internal states of adhesion molecules are coupled to their aggregation dynamics sufficiently strongly, the system becomes instable and unbounded growth ensues. Unexpectedly, the very same type of instability can lead to perfect stability under mechanical load, where adhesions adapt their size to withstand arbitrarily large load without rupturing-a phenomenon we term perfect stabilization. We derive state diagrams characterizing adhesion stability under stationary load and show that perfect stabilization also occurs for dynamic loads on physiologically relevant timescales. Finally, we show that perfect stabilization is a generic phenomenon that can be realized in many different ways by coupling aggregation rates with internal molecular states and argue that the phenomenon has broad implications for understanding cellular mechanics.

BP 25.3 Thu 10:15 H44

Environmental stiffness regulates neuronal maturation via Piezo1-mediated TTR activity — •Eva Kreysing[1,2,3], Hélène Gautier[1], Leila Muresan[1], Sudipta Mukherjee[1,2,3], Alexander Winkel[1], Xiaohui Zhao[1], Ragnhildur Thóra Káradóttir[1], and Kristian Franze[1,2,3] — [1]University of Cambridge, UK — [2]FAU Erlangen — [3]MPZ Erlangen

During the development of the nervous system, neurons grow axons and dendrites to connect with other cells. As neurons become integrated into the neural network, they mature and develop electrical activity. While mechanical interactions between neurons and their environment are critical for axon growth and pathfinding, the role of mechanical cues in the electrical maturation of neurons, and thus the formation of circuits in the developing brain, remain unexplored. Here, we cultured rat hippocampal neurons on substrates with different mechanical properties and found that electrical activity developed earlier on soft hydrogels compared to stiff hydrogels. This stiffness-dependent neuronal maturation was mediated by the mechanosensitive ion channel Piezo1. Using RNA sequencing, pathway analysis and Western blots, we identified a downstream signalling cascade responsible for the differential expression of neurotransmitter receptors. Finally, we found that stiffening of the developing Xenopus brain leads to impaired synapse formation in vivo. Our findings highlight the critical role of mechanical signals in neuronal maturation and suggest that local brain tissue stiffness is a critical parameter for circuit formation in the developing brain.

BP 25.4 Thu 10:30 H44

The positioning of stress fibers in contractile cells minimizes internal mechanical stress — •Valentin Wössner[1,2], Lukas Riedel[3,4], Dominic Kempf[3], Falko Ziebert[1,2], Peter Bastian[3], and Ulrich S. Schwarz[1,2,3] — [1]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany — [2]BioQuant, Heidelberg University, Heidelberg, Germany — [3]Interdisciplinary Center for Scientific Computing, Heidelberg University, Heidelberg, Germany — [4]Institute for Environmental Decisions, ETH Zürich, Zürich, Switzerland

Stress fibers are contractile bundles of actin filaments found in the cytoskeleton of animal cells. They play crucial roles in force generation, mechanical adaptation, shape control and mechanosensing. While the physical description of single stress fibers is well-developed, much less is known about their spatial distribution on the level of whole cells. Here, we combine a finite element method for one-dimensional fibers embedded in a two-dimensional elastic bulk medium with dynamical rules for stress fiber formation based on genetic algorithms [1]. We postulate that their main goal is to achieve minimal mechanical stress in the bulk material with as few fibers as possible. We find that stress

fibers typically run through the cell in a diagonal fashion and that they cross each other under biaxial stretch. In the future, our approach can be extended to three dimensions and to stress fibers with viscoelasticity.

[1] Riedel et al., J. Mech. Phys. Solids 195 (2025) 105950

BP 25.5 Thu 10:45 H44

Towards a better understanding of the cytokinetic contractile ring — •Francine Kolley-Köchel[1] and Sebastian Aland[1,2] — [1]Faculty of Mathematics and Informatics, TU Freiberg, 09599 Freiberg, Germany — [2]Faculty of Informatics/Mathematics, HTW Dresden, 01069 Dresden, Germany

The dynamics of viscoelastic surfaces plays an important role in biological systems. One prominent example is the actin cortex, with elastic properties on short time scales and viscous on long time scale. Numerical simulations of such a system can provide a better understanding of the real biological system. Here we present a novel monolithic model of viscoelastic surfaces within a dominant surface rheology, capturing both, shear and dilational dynamics. We demonstrate that these full three dimensional simulations are numerically stable for low and high surface viscosities and show spontaneous pattern formation, induced by active stress regulation. We discuss how this model can guide future work towards a betters understanding of complex viscoelastic surface dynamics and the formation of the cytokinetic contractile ring.

BP 25.6 Thu 11:00 H44

Using microfluidics for measuring microplastic particle-cell interactions — •Matteo A. Kumar[1], Simon Wieland[1,2], Anja F.R.M. Ramsperger[1,2], Christian Laforsch[1,2], and Holger Kress[1] — [1]Biological Physics, University of Bayreuth, Germany — [2]Animal Ecology I and BayCEER, University of Bayreuth, Germany

The growing presence of microplastic particles (MPs) in the environment increases human exposure to these contaminants, which can accumulate in tissues and spread throughout the body. Various MP properties, such as shape, size, charge and surface morphology, influence their interactions with cells. We have recently shown that the zeta-potential of MPs significantly affects their adhesion to and internalization into cells*. However, the question, whether the zeta-potential directly or another underlying parameter influencing it (e.g. the number of functional surface groups) plays the decisive role, remains unsolved.

To address this, we use a microfluidic platform and combine it with a convolutional neural network to allow the measurement of hundreds of interactions in parallel. By allowing MPs with different surface functionalizations to sediment onto the cells, we determine their binding kinetics. We subsequently exert a well-defined flow force on the MPs to quantify their adhesion to the cells. Our work contributes to understanding which properties of MPs are determining particle-cell interaction and therefore identifying potential drivers for their biological impact.

*Wieland, S., Ramsperger, A.F.R.M., Gross, W. et al. Nat Commun 15, 922 (2024).

15. min. break

BP 25.7 Thu 11:30 H44

Direct mechanical communication of cellular to nuclear shape in oocytes — •Bart Vos[1], Yamini Vadapalli[2], Till Muenker[1], Peter Lenart[2], and Timo Betz[1] — [1]Third Institute of Physics, University of Göttingen, Göttingen, Germany — [2]Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

Mechanics play a crucial role in a wide range of cellular processes, from differentiation to division and metastatic invasion. Additionally, mechanical signaling can regulate protein expression. Although the mechanical properties of the cytoskeleton, providing shape, motility and mechanical stability to the cell, have been extensively studied, remarkably little is known about the mechanical environment within the nucleus of a cell and the exact mechanisms of force transduction between the cytoplasm to the nucleus.

To address these questions, we apply external deformations to oocytes of different species to observe how cellular deformations can be transmitted to the nucleus, leading to nuclear deformations. We combine this with optical tweezers-based microrheology in the cellular nucleus, allowing a direct comparison between intracellular and intranuclear mechanics. The observed viscoelastic behavior of the nucleoplasm on various time scales is profoundly different from the cytoskeleton. In addition, we probe the role of activity in the mechanics of the nucleus. Depending on the mechanical properties of the cytoplasm and nucleoplasm, nuclei can be highly susceptible to external strain or be largely shielded, suggesting a mechanical communication that might be relevant for proper oocyte function.

BP 25.8 Thu 11:45 H44

Robust mitotic events in C. elegans embryos with and without mechanical perturbations — Vincent Borne and •Matthias Weiss — Experimental Physics I, University of Bayreuth, Germany

Early embryogenesis of the nematode Caenorhabditis elegans proceeds in an autonomous fashion within a protective chitin eggshell. Cell-division timing and the subsequent mechanically guided positioning of cells is virtually invariant between individuals, especially before gastrulation. By mechanically perturbing the embryo without breaking its eggshell, we have probed the limits of this stereotypical and robust developmental program. Compressing embryos to half of their native diameter frequently resulted in a loss of cytokinesis, yielding a non-natural syncytium that still allowed for multiple divisions of nuclei. The orientation of mitotic axes was strongly altered in the syncytium, but key features of division timing and spatial arrangement of nuclei remained surprisingly similar to those of unperturbed embryos in the first few division cycles. Our data suggest that few very robust mechanisms govern the progress of early embryogenesis of C. elegans.

BP 25.9 Thu 12:00 H44

Density and viscosity Measurements of the cytosol of human red blood cells — •Thomas John and Christian Wagner — Experimental Physics, Saarland University

We present a method to determine the viscosity of the intracellular liquid - the cytosol - of human red blood cells (RBCs). Our method combines the measurement of the mass density distribution of RBCs and the viscosity of the cytosol as a function of the water content. The density distribution is measured through buoyant density centrifugation combined with cell counting. By correlating this Gaussian distribution of cell population densities with the viscosity-density relation of the cytosol, we obtain a log-normal distribution of the cytosol viscosity of healthy RBCs. The viscosity contrast λ, defined as the ratio of viscosities between the RBC cytosol and the blood plasma under physiological conditions, is determined to have a mean value of $\bar{\lambda} = 10$. This value is significantly larger than those used in the literature for numerical simulations.

BP 25.10 Thu 12:15 H44

Aggregation and disaggregation of red blood cells — •Kirill Korneev[1], Nicolas Moreno[2], Thomas John[1], Christian Wagner[1], and Dmitry Fedosov[3] — [1]Experimental Physics, Saarland University — [2]Basque Center for Applied Mathematics, Bilbao Spain — [3]Theoretical Physics of Living Matter, Forschungszentrum Jülich

Laser tweezers (LT) are devices for manipulating, trapping and force measurement on particles into optical traps. Red blood cells (RBCs) are the majority of blood cells. Those cells are very deformable and show spontaneously forming complex structures at rest state, due to aggregation. The mechanisms of RBCs aggregation are not fully understood, however there are currently two main hypotheses that can explain it: the bridging model based on mobile and immobile bonds, and the depletion layer model. In this work, experimental values of the RBCs disaggregation force were obtained by stretching RBC aggregates. We will show, that the mechanism of RBCs disaggregation involves these two hypotheses. We will also show that the bridging model with mobile bonds reproduces well the corresponding experimental data, offering insights into the interplay between bridging and depletion interactions and providing a framework for studying similar interactions between other biological cells.

N. Moreno, et al., Aggregation and disaggregation of red blood cells: depletion versus bridging, bioRxiv 2024.11.20.624311 (2024)

BP 25.11 Thu 12:30 H44

Dynamic states of P. falciparum infected erythrocytes adhering in shear flow - a qualitative study of rolling and flipping motions — •Katharina Scholz[1], Leon Lettermann[2], Jessica Kehrer[3], Michael Lanzer[3], Ulrich Schwarz[2], and Motomu Tanaka[1] — [1]Institute for Physical Chemistry, University of Heidelberg, Germany — [2]Institute for Theoretical Physics, University of Heidelberg, Germany — [3]Center of Infectious Diseases, Heidelberg University Medical School, Germany

As surviving strategy, the malaria parasite remodels the red blood cell by causing the expression of adhesive proteins on its surface. The modification allows the infected cell to adhere to the endothelial cells in the blood stream, thereby avoiding clearance by the spleen.

This transformation also alters cell shape and movement behaviour during development. We used Reflection Interference Contrast Microscopy (RICM) in quantitative flow chamber experiments and employed a high-speed camera to gain more information about the contact footprint of cells. With this setup, we tracked parasitised erythrocytes individually, label-free and non-invasively. Early-stage trophozoites exhibited flipping behaviour, while late-stage schizonts showed a steady rolling motion. Our results provide a quantitative understanding of how parasite development affects dynamic cytoadhesion behaviour and shed light on understanding endothelial cell activation.

BP 25.12 Thu 12:45 H44

Deformability cytometry for large-scale mechano-genomic screening in interphase and mitosis — •Laura Strampe[1], Katarzyna Plak[2,3], Christine Schweitzer[1], Cornelia Liebers[1,2], Buzz Baum[3], Jona Kayser[1], and Jochen Guck[1,2] — [1]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [2]Biotechnology Center of TU Dresden, Dresden, Germany — [3]MRC Laboratory of Molecular Biology, Cambridge, United Kingdom

We demonstrate the scalability of real-time fluorescence and deformability cytometry (RT-FDC) for large-scale cell cycle-resolved mechano-genomic screening. Using RNA interference, we screened 215 kinase and phosphatase genes on their effects on cell mechanics in interphase and mitosis. RT-FDC combines high throughput (up to 100 cells per second) with fluorescence-based cell cycle classification, enabling single-cell mechanical phenotyping of entire populations. We show that cell cycle resolution is essential for identifying genetic regulators of cell mechanics, as stiffness differences between interphase and mitotic cells can obscure genuine knockdown effects or generate false-positive hits. Genes regulating mitotic mechanics or softening cells upon knockdown are particularly likely to be masked. Of the 81 genes identified as affecting cell stiffness, 22 were detected only through cell cycle resolution. These include *PRL-1*, a cancer metastasis marker with opposing effects across the cell cycle: stiffening interphase cells and softening mitotic cells. This suggests that *PRL-1* overexpression in metastatic cells expands the range of mechanical phenotypes during cell cycle progression, facilitating tumor adaptability.

BP 26: Synthetic life-like systems and Origins of Life

Time: Thursday 9:30–12:15 Location: H46

BP 26.1 Thu 9:30 H46

Heat flows through rock cracks purify life's building blocks and protect RNA from hydrolysis — •Paula Aikkila[1], Thomas Matreux[2], Dieter Braun[1], and Christof Mast[1] — [1]Ludwig-Maximilians-Universität München — [2]ESPCI Paris

The emergence of biopolymer building blocks is a crucial step during the origins of life. However, their synthesis pathways usually require feedstocks of pure reactants and defined purification and mixing steps to suppress unwanted side reactions, which is required for high product yields. We show that heat flows through thin crack-like compartments purify complex mixtures of prebiotically relevant building blocks and drive prebiotically relevant reactions such as the dimerization of glycine. In these same compartments, we furthermore study how heat-flows can locally switch on and off pH gradients, thereby enabling or disabling RNA hydrolysis depending on their hybridization state. We seek to explore how this enables spontaneous symmetry breaking in the sequence and folding space, possibly facilitating the emergence of functional ribozyme.

BP 26.2 Thu 9:45 H46

Membraneless protocell confined by a heat flow — •Alexander Floroni[1], Noël Yeh Martín[2], Thomas Matreux[1], Laura Weise[3], Sheref Mansy[4], Hannes Mutschler[5], Christof Mast[1], and Dieter Braun[1] — [1]Systems Biophysics, LMU Munich; München, Germany — [2]Institute of Biotechnology HiLIFE, University of Helsinki, Helsinki, Finland — [3]MPI of Biochemistry; Martinsried, Germany — [4]Department of Chemistry, University of Alberta; Edmonton, Canada — [5]Department of Chemistry and Chemical Biology, TU Dortmund; Dortmund, Germany

In living cells, a complex mixture of biomolecules is assembled within and across membranes. This state is maintained by a sophisticated protein machinery. It imports nutrients, removes waste, and orchestrates cell division. Here we show how the molecular contents of a cell can be coupled in a coordinated way to the non-equilibrium of a heat flow. A temperature difference across a water-filled pore accumulated the core components of a modern cell to make a functional reaction. The mechanism arose from the interplay of convection and thermophoresis. Protein synthesis was triggered as a direct result of the up-concentration. The same non-equilibrium setting continued to attract nutrients from an adjacent fluid stream, while keeping the cellular molecules confined. Our results show how a simple and archaic non-equilibrium physical process can assemble the many different molecules of a cell and trigger its basic functions. The framework provides a membrane-free environment to bridge the long evolutionary times from an RNA world to a protein-based cell-like proto-metabolism.

BP 26.3 Thu 10:00 H46

A game of life with dormancy — •Daniel Henrik Nevermann[1], Claudius Gros[1], and Jay Lennon[2] — [1]Institute for Theoretical Physics, Goethe-University Frankfurt, Germany — [2]Department of Biology, Indiana University, Bloomington, IN 47405, USA

The factors contributing to the persistence of life are fundamental for understanding complex living systems. Many species contend with harsh environments by entering a reversible state of reduced metabolic activity, a phenomenon known as dormancy. Here, we develop Spore Life, a model to investigate the effects of dormancy on population dynamics. It is based on Conway's Game of Life, a deterministic cellular automaton where simple rules govern the metabolic state of an individual based on its neighborhood. For individuals that would otherwise die, Spore Life provides a refuge in the form of an inactive state. These dormant individuals (spores) can resuscitate when local conditions improve. The model includes a parameter $\alpha \in [0, 1]$ that controls the survival probability of spores, which yields stochastic dynamics between the limits $\alpha = 0$ (Game of Life) and $\alpha = 1$ (Spore Life). In addition to identifying the emergence of unique periodic configurations, we find that spore survival increases the average number of active individuals and buffers populations from extinction. Contrary to expectations, the population stabilization does not require large and long-lived seed bank. Instead, the demographic patterns in Spore Life only require a small number of resuscitation events. Spore Life can be interactively explored at `https://itp.uni-frankfurt.de/spore-life/`.

BP 26.4 Thu 10:15 H46

Continuous Evolving Game of Life with Diversity — •Alexandre Guillet and Frank Jülicher — MPI-PKS, Dresden, Germany

The complex phenomenology of J. Conway's "Game of Life" cellular automaton, in particular its gliders, has been translated into continuous fields in space and time in a 2011 preprint by S. Rafler. The striking organic feel associated with these artificial life simulations in isotropic space has attracted the attention of a growing online community at the intersection of citizen science and computer art, which has recently culminated in the exploration and classification of the diverse morphologies of the "Lenia" gliders by BWC. Chan and others.

Our research focuses on a minimal variant of these continuous nonlinear dynamical systems that is capable of generating gliding, self-replicating and vanishing patterns, with striking resemblance to cell division, motility and death. Elaborating upon the governing partial integro-differential equation, we allow each cell to carry individual variations of the parameters, thus introducing a spatial diversity of rules. A conservation law is enforced on the resources of the cells as a selection pressure, together with a mutation process as a random source of diversity. The spontaneous evolution of the system from a single cell leads to a rich phenomenology, ranging from mycelial growth to epithelia and amoeboid motion.

This continuous and evolving model with diversity raises the Game of Life into a toy model for the morphogenesis and evolution of primordial lifeforms.

BP 26.5 Thu 10:30 H46

Cooperative effects in compartmentalized irreversible self-assembly — •Richard Swiderski, Severin Angerpointner, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Germany

From biomolecular compartments, protein patterns to porous rocks: Many biological and chemical systems like living cells or prebiotic chambers exhibit some form of spatial organization which separates biochemical processes. This is known to play a key role in the assembly of virus capsids or the enrichment of prebiotic chemicals. We systematically explore the effects of such spatial separation on the self-assembly of irreversibly binding identical particles. We show that already in a simplified model of two coupled biochemical compartments cooperative effects emerge through limiting compartment exchange. Further, these findings generalize to spatially extended systems like intracellular chemical gradients or membrane-assisted assembly.

15 min. break

Invited Talk BP 26.6 Thu 11:00 H46

Theory for sequence selection via phase separation and oligomerization — •Christoph Weber — University of Augsburg, Universitätsstr. 1, 86159 Augsburg

Non-equilibrium selection pressures were proposed for the formation of oligonucleotides with rich functionalities encoded in their sequences, such as catalysis. Since phase separation was shown to direct various chemical processes, we ask whether condensed phases can provide mechanisms for sequence selection. To answer this question, we use non-equilibrium thermodynamics and describe the reversible oligomerization of different monomers to sequences at non-dilute conditions prone to phase separation. We find that when sequences oligomerize, their interactions give rise to phase separation, boosting specific sequences' enrichment and depletion. Our key result is that phase separation gives rise to a selection pressure for the oligomerization of specific sequence patterns when fragmentation maintains the system away from equilibrium. Specifically, slow fragmentation favors alternating sequences that interact well with their environment (more cooperative), while fast fragmentation selects sequences with extended motifs capable of specific sequence interactions (less cooperative). Our results highlight that out-of-equilibrium condensed phases could provide versatile hubs for Darwinian-like evolution toward functional sequences, both relevant for the molecular origin of life and de novo life.

BP 26.7 Thu 11:30 H46

Prebiotic RNA Replication through Templated Ligation by Humidity and pH Cycles — •Felix T. Dänekamp and Dieter Braun — Systems Biophysics LMU, Munich, Germany

To replicate long RNA strands, templated ligation from 2',3'-cyclic phosphate RNA is a promising pathway. Preliminary screenings suggest that through tuning of monovalent salt content and through adding Lysine or other amino acids to the solution, no additional catalysts are required to attain yields of 50% ligation product in one day. Cycling physical conditions such as pH and salt/RNA concentration likely solves the strand inhibition problem. This opens up the possibility of prebiotic ligation chain reactions and thus open-ended evolution from short RNA strands.

BP 26.8 Thu 11:45 H46

Gravitationally induced oscillations of active droplets — •Advait Thatte[1], Judit Sastre[2], Alexander Bergmann[2], Michele Stasi[2], Marta Tena-Solsona[2], Job Boekhoven[2], and Christoph Weber[1] — [1]Faculty of Mathematics, Natural Sciences, and Materials Engineering, and Institute of Physics, University of Augsburg, Universitätsstrasse 1, 86159 Augsburg, Germany — [2]Department of Bioscience, School of Natural Sciences, Technical University of Munich, Lichtenbergstrasse 4, 85748 Garching, Germany

Oscillations in the formation and dissolution of compartments inside living cells are pivotal in orchestrating various cellular functions and processes. Recent experiments on synthetic cells showed the spontaneous emergence of spatio-temporal oscillations in the number of droplets, their size, and position. Oscillations occur because droplets grow via gravitationally induced fusion above their stationary size. As a result droplets shrink, feeding the nucleation of new sedimenting droplets, restarting the cycle. The stationary droplet size is a consequence of deactivating droplet material inside and activating outside. Here we present a theoretical model for phase separation with non equilibrium chemical fuelling including a sharp interface model for many active droplets. The model quantitatively describes the stationary droplet size and the oscillation frequency observed experimentally.

BP 26.9 Thu 12:00 H46

Linking fitness landscape topography to the characteristics of the underlying genotype-phenotype map — Malvika Srivastava[1,2], Ard A. Louis[3], and •Nora S. Martin[4] — [1]Institute of Integrative Biology, ETH Zurich, Zurich, Switzerland — [2]Swiss Institute of Bioinformatics, Lausanne, Switzerland — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, UK — [4]CRG (Barcelona Collaboratorium for Modelling and Predictive Biology), Dr. Aiguader 88, Barcelona 08003, Spain

The topographies of fitness landscapes are central in models of evolutionary processes. Key topographical features include the prevalence of fitness peaks, as well as the existence of accessible (i.e. fitness-increasing) paths to the global fitness optimum. Recent numerical work found that such accessible paths commonly exist in fitness landscapes based on biophysical models of genotype-phenotype (GP) maps, even when fitness values are randomly assigned to phenotypes [1]. Here, we examine such landscapes with random phenotype-fitness assignment more thoroughly to investigate, how their topography depends on the characteristics of the underlying GP map. By simplifying the GP map to a "neutral component" (NC) graph, we can compute the expected prevalence of fitness peaks based only on two GP map characteristics: the evolvabilities and sizes of NCs. Evolvabilities are also important for peak heights and for the existence of accessible paths to global optima. [1] S. F. Greenbury, A. A. Louis, S. E. Ahnert, Nat Ecol Evol. 6, 1742-1752 (2022).

BP 27: Focus Session Chemical Imaging for the Elucidation of Molecular Structure I (joint session O/BP)

Unravelling the multiscale molecular heterogeneity at interfaces is one of the main challenges in modern biophysics and surface science due to the major role specific structural properties play in determining their macroscopic function and behavior. In the last few decades, several specialized chemical imaging techniques have been developed that can reveal many of these crucial structural details, representing an enormous advance in our elucidative capabilities. Clear examples of this range from super-resolution and 3D tomography to tag-free characterization down to the single-molecule level. This focus session will explore the vast range of methods and possibilities for characterizing the different structural aspects in heterogeneous molecular systems and specifically highlight the potential complementarity of the different techniques through multi-modal approaches. Overall, by bringing together different communities, this session aims to foster scientific exchanges that could spark the next major developments in chemical imaging.

Organized by
Martin Thämer (FHI Berlin), Alexander Fellows (FHI Berlin), and Kerstin Blank (University Linz)

Time: Thursday 15:00–17:30 Location: H24

Invited Talk BP 27.1 Thu 15:00 H24

Infrared Nanoscopy and Tomography of Intracellular Structures — Joachim Heberle[1], Katerina Kanevche[1], •Emmanuel Pfitzner[1], David Burr[2], Janina Drauschke[2], Andreas Elsaesser[2], and Jacek Kozuch[1] — [1]Freie Universität Berlin, Department of Physics, Experimental Molecular Biophysics, — [2]Experimental Biophysics and Space Sciences, Arnimallee 14, 14195, Berlin, Germany

Although techniques such as fluorescence-based super-resolution imaging or confocal microscopy simultaneously gather morphological and chemical data, these techniques often rely on localized and chemically specific markers. To eliminate this flaw, we have developed a method of examining cellular cross-sections using the imaging power of scattering-type scanning near-field optical microscopy (sSNOM) and Fourier-transform infrared spectroscopy at a spatial resolution far beyond the diffraction limit (nanoFTIR). Herewith, nanoscale surface and volumetric chemical imaging are performed using the intrinsic contrast generated by the characteristic absorption of mid-infrared radiation by the covalent bonds. We employ infrared nanoscopy to study the subcellular structures of eukaryotic (C. reinhardtii) and prokaryotic (E. coli) species, revealing chemically distinct regions within each cell. Serial 100 nm-thick cellular cross-sections were compiled into a tomogram, yielding a three-dimensional infrared image of subcellular structure distribution at 20 nm spatial resolution. The presented methodology can image biological samples with less interference due to the low energy of infrared radiation and the absence of labeling.

Invited Talk BP 27.2 Thu 15:30 H24

Coherent Raman Imaging — •Michael Schmitt[1] and Juergen Popp[1,2] — [1]Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller-University Jena, Helmholtzweg 4, 07743 Jena, Germany — [2]Leibniz Institute of Photonic Technology, Member of Leibniz Health Technologies, Albert-Einstein-Straße 9, 07745 Jena, Germany

Raman-based technologies have profoundly impacted life sciences and biomedical research. Despite their unmatched molecular specificity, traditional Raman spectroscopy suffers from limited sensitivity, making it less suitable for rapid imaging. This limitation is addressed by coherent Raman scattering (CRS) microscopy, primarily through coherent anti-Stokes Raman scattering (CARS) and stimulated Raman scattering (SRS). This talk examines the potential of CARS and SRS imaging for biological and biomedical analysis, offering detailed insights into the molecular composition of biomedical specimens, such as cells or tissue. The presentation will focus on the applications of these techniques in molecular and functional diagnostics in the fields of medicine and life sciences. Furthermore, recent developments in translating CRS into compact, clinically viable systems, such as handheld probes, will be presented, focusing on intraoperative tumour diagnostics for early detection and improved improved therapeutic outcomes.

Acknowledgement: Financial support of the EU, the *Thüringer Ministerium für Wirtschaft, Wissenschaft und Digitale Gesellschaft*, the *Thüringer Aufbaubank*, the BMBF, the DFG, and the Carl Zeiss Stiftung is acknowledged.

Invited Talk BP 27.3 Thu 16:00 H24

Sum Frequency Generation Microscopy of Electrochemical Interfaces — •Steven Baldelli — University of Houston, Houston, Texas

Sum frequency generation spectroscopy (SFG) is a valuable technique to study the molecular properties of surfaces. As a second-order technique, it is uniquely sensitive to the average organization of molecules at the surface. However, as most surfaces are spatially heterogeneous, it isn't easy to interpret the spectrum as a single domain. The development of SFG into microscopy has allowed a more detailed and accurate analysis of the spatio-spectro-temporal evolution of surface chemistry. The SFG microscope development will be presented, and compressive sensing and the application toward electrocatalysis will be used.

BP 27.4 Thu 16:30 H24

Elucidating the Composition, Order, and 3D Molecular Orientation of Thin Films with Phase-Resolved Sum-Frequency Generation Microscopy — •Alexander Fellows, Ben John, Martin Wolf, and Martin Thämer — Fritz-Haber-Institute, Berlin, Germany

The vast majority of molecular interfaces have highly heterogeneous structures, ranging across all length-scales. These manifest as variations in density, composition, and molecular packing structure, all of which are critical in controlling the macroscopic properties and functional behaviour of the films. While various chemical imaging techniques can access many of these important structural details, characterising their relative order and specific packing arrangements represents a formidable challenge.

Here, we present a chemical imaging approach based on phase-resolved sum-frequency generation (SFG) microscopy. By probing molecular vibrations, this technique achieves molecular recognition and thus is sensitive to the local composition and density. Furthermore, through its symmetry selection rules, output SFG signals are dependent on absolute molecular orientations. This hence allows it to distinguish different molecular conformations and characterise the amount of orientational order in the system. Finally, with an azimuthal-scanning approach, the in-plane and out-of-plane signal contributions can be separated, allowing the 3D molecular orientations to be elucidated. By applying SFG imaging to model lipid monolayers, we gain an unprecedented overview of their hierarchical packing structures.

BP 27.5 Thu 16:45 H24

Low temperature multimode atomic force microscopy using an active MEMS cantilever — Michael G. Ruppert[1], Miguel Wiche[2], André Schirmeisen[2], and •Daniel Ebeling[2] — [1]University of Technology Sydney, Australia — [2]Justus Liebig University Giessen, Germany

Low-temperature atomic force microscopy (AFM) is one of the most powerful tools in surface science. With the chemical bond imaging technique, i.e., by using CO functionalized AFM tips, it became possible to visualize the chemical structure of individual organic molecules, which is essential for studying on-surface reactions and molecular manipulation processes. Routinely, such measurements are performed

with qPlus sensors. Here, we present a proof of concept for an active microelectromechanical systems (MEMS) microcantilever with integrated piezoelectric sensing and demonstrate its capability to obtain scanning tunneling microscopy as well as high-resolution non-contact atomic force microscopy images on an atomically flat Au(111) surface. Equipped with a focused ion beam deposited tungsten tip, the active MEMS cantilever is able to obtain high contrast scanning tunneling and frequency shift images at the fundamental and a higher eigenmode of the cantilever. This is interesting for the application of multifrequency AFM operation modes that could enhance the capabilities of the bond imaging technique.

BP 27.6 Thu 17:00 H24

Instrumentation for high-resolution biomolecule imaging enabled by electrospray ion beam deposition (ES-IBD) — •Lukas Eriksson[1], Tim Esser[1,2], and Stephan Rauschenbach[1] — [1]University of Oxford, Oxford, UK — [2]Thermo Fisher Scientific, Eindhoven, Netherlands

Direct imaging of (bio-)molecules with cryogenic electron microscopy (cryo-EM) or scanning probe microscopy (SPM) is a powerful approach for elucidating molecular structure. However, sample preparation can be a major challenge: either very time- and resource-intensive or incompatible with the vacuum environment required by the imaging method.

Here, we explore preparative mass spectrometry as an alternative workflow towards structural elucidation of biomolecules. A novel, custom-built deposition stage extending a commercial mass spectrometer (Thermo Fisher Scientific Orbitrap UHMR) allows for the mass-filtered, soft-landed deposition of a wide mass range of target molecules (m = 100 to 10^6 Da) onto various surfaces, including cryo-EM grids and metal crystals for SPM. Successful deposition and subsequent imaging requires extensive control over conditions such as pressure, temperature, ion trajectories, sample surfaces, and sample transfer to obtain clean, chemically pure samples of the desired species in the right (i.e. native) configuration. The sample holder also enables controlled growth of ice layers for embedding deposited molecules, allowing high-resolution reconstructions of proteins from cryo-EM.

BP 27.7 Thu 17:15 H24

LFM study of copper oxide — •Sophia Schweiss, Alfred J. Weymouth, and Franz J. Giessibl — Universität Regensburg, Regensburg, Deutschland

Small-amplitude FM-AFM is a method to study surfaces and adsorbates with atomic resolution. At low temperature, the tip apex can be prepared so that it ends in a single O-atom, making the tip inert and enhancing imaging [1, 2]. With a laterally oscillating tip, i.e. lateral force microscopy (LFM), the conservative (frequency shift, Δf) and non-conservative (dissipated energy, E_{diss}) components of the tip-sample interaction can also be independently measured. Here too, inert tip apices are commonly used. One measurement of E_{diss} relies on the cocking and snapping of the tip over a single chemical bond, for which the current state of the art utilizes CO-terminated tips. In this work, a CO-terminated tip [1] is used to investigate the (2×1)O reconstruction of Cu(110) with LFM. Simulations are performed to guide interpretation. In this larger ongoing study, these LFM measurements will be repeated for a CuOx tip [2] to evaluate it as a tool for measuring E_{diss}.

[1] Gross et al., Science, **325**, 1110 (2009)
[2] Mönig et al., Nat. Nano., **13**, 371 (2018)

BP 28: Microswimmers and Microfluidics (joint session DY/BP/CPP)

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

Invited Talk BP 28.1 Thu 15:00 H37

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

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

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

BP 28.2 Thu 15:30 H37

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

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

BP 28.3 Thu 15:45 H37

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

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

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

BP 28.4 Thu 16:00 H37

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

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

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

BP 28.5 Thu 16:15 H37

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

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

15 min. break

BP 28.6 Thu 16:45 H37

Corrugated channels can filter ciliated microorganisms based on the metachronal wavelength — •Gonçalo Antunes and Holger Stark — Technische Universität Berlin, Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Many microorganisms (e.g. Paramecium) move by a carpet of cyclically beating cilia that cover their surface. These cilia often beat in an organized fashion, such that the beating phases form a traveling wave, referred to as a metachronal wave. In this study, we investigate the swimming of such microorganisms in corrugated microchannels. We model the motion of the cilia via a time-varying effective slip velocity applied on the microorganism's surface, which we approximate as an infinite slab. By employing the lubrication approximation, we show analytically that the swimming speed of ciliated microorganisms placed inside a corrugated channel is sensitive to the corrugation height, provided that the wavelength of the corrugation matches that of the metachronal wave. Indeed, the direction of motion itself may invert with respect to swimming in bulk fluid, with the channel acting as a virtual barrier which blocks microorganisms under specific conditions for corrugation and slip-velocity modulations, but allow others to pass through. We also show that the interplay between the corrugation and the slip velocity profile allows for the swimming of microorganisms with zero time-averaged slip velocity, which thus cannot swim in bulk fluid. Finally, we complement our theory with preliminary results from hydrodynamic simulations for radially-symmetric microorganisms of finite length in radially-symmetric corrugated channels.

BP 28.7 Thu 17:00 H37

Motion of a single particle partially exposed in a simple shear flow — •Dominik Geyer[1,2], Aouane Othmane[1], and Jens Harting[1,2] — [1]Helmholtz-Institut Erlangen-Nürnberg for Renewable Energy (IET-2), FZ Jülich — [2]Department of Physcis, FAU Erlangen-Nürnberg

Sand immersed in the water can be imagined as a wet granular matter. Besides sedimentation, friction, and surface roughness are two relevant physical phonemes within this system. Many body systems in a turbulent regime have been studied using discrete elements methods for a long time, but a single particle in the Stokes flow regime is particularly interesting for biological systems and microfluidic devices.

A layer of quadratic-arranged spheres models the rough surface. The question arises of how to describe the motion of a single traveling particle over this substrate.

We choose a combined numerical and analytical approach. The Stokes equation is solved analytically for the sphere near a rough wall. Lattice Boltzmann simulations with momentum-exchange particle coupling are performed for different wall roughness and friction coefficients.

Although, the Stokes equation assumes that the particle Reynolds number is zero. Surprisingly, the numerical results match our theoretical description until a particle Reynolds number of two. In this regime, friction between the moving particle and the substrate significantly influences the angular velocity but has a minor influence on the traveling velocity in the flow direction.

BP 28.8 Thu 17:15 H37

Rational Design of Smart Microfluidics in Responsive Channels — •Arwin Marbini — Albert-Ludwigs Universität Freiburg

Responsive microfluidics offers exciting potential for self-regulating biomimetic systems. This study explores bifurcating microchannel networks with pressure-sensitive resistances, combining experiments with simulations based on the Hagen-Poiseuille equation and a linear model. These methods extract critical, experimentally inaccessible parameters under steady-state and dynamic conditions. Our findings enable the design of adaptable microfluidic networks, unlocking precise flow control for future applications in biology, soft robotics, and advanced material systems.

BP 28.9 Thu 17:30 H37

Blue Water: A passive, reusable microfiltration device for water purification — •Tim R. Baumann, Ioannis Gkekas, Martina Viefhues, and Dario Anselmetti — Experimental Biophysics, Bielefeld University

Water is the most vital resource for life on Earth. Due to pollution of freshwater and oceans, this valuable resource has become globally endangered. The effects of microplastic pollution are widely discussed in scientific, political, and socioeconomic contexts. Despite regulations on single-use plastics and microplastic output, efforts should also focus on reintegrating microplastics to achieve a sustainable circular economy. Furthermore, microplastic-sized particles can migrate through organic tissue and can therefore be classified as contaminants of emerging concern. However, filtering plastics of this size is a challenging task.

Thus, this work examines and extends the findings of Divi et al. regarding the suspension feeding mechanisms of various ray species. We studied the filtration performance and efficiency for different geometric ratios of channel widths in simulations and laboratory environments. First, we have the main inner channel connected to the pressure inlet. From this, two rows of tilted lamellae structures branch off laterally to the outer secondary channels.

By applying sufficiently high pressure ($> 6 \cdot 10^5\ Pa$) to the inlet and achieving flow and particle velocities of $> 35\ \frac{m}{s}$, we can purify 82 % of half of the initial fluid. To prevent rupturing of our microfluidic chip under this pressure, we further investigated using glass fiber reinforced PDMS and lowering the operating pressure.

BP 29: Focus Session: Innovations in Research Software Engineering (joint session BP/DY)

Research software engineering (RSE) is an emerging field in science, with practitioners spanning a continuous spectrum from "researchers who code" to "software engineers developing for science". In Germany, a growing movement supported by deRSE e.V. is gaining recognition, and more institutions are acknowledging the increasing demand across various disciplines. This focus session will provide a platform to highlight recent advances in applications, tooling, and software in the fields of biophysics, dynamics, and statistical physics, as well as developments in the recognition and proliferation of RSE as a profession within our field and academia in general.

Organized by Simon Christ and Sophia Rudorf (Hannover).

Time: Thursday 15:00–18:00 Location: H44

Invited Talk BP 29.1 Thu 15:00 H44

Community-driven software and data training for computational biology — •Toby Hodges — The Carpentries, Oakland, CA, USA

The Carpentries is a global community teaching essential software and data skills for research. Certified Instructors teach hundreds of workshops to thousands of learners all over the world every year, introducing them to essential skills for computational research such as programming, version control, and data organisation. In recent years, the community has also begun to develop and deliver lessons that build on these foundations, teaching more intermediate and advanced Research Software Engineering skills such as HPC, parallel programming, and containerised computing. This talk will explore how open source, collaborative training efforts can build capacity for computational research, discuss what makes this model work and some lessons learned along the way, and finish with a look at what the community plans to do next.

BP 29.2 Thu 15:30 H44

Python-based interface to micromagnetic simulation software: Ubermag — •Hans Fangohr[1,2,3], Martin Lang[1,2], Samuel J.R. Holt[1,2], Swapneel Amit Pathak[1,2], Kauser Zulfiqar[1,2,4], and Marijan Beg[5] — [1]MPSD, Hamburg, Germany — [2]CFEL, Hamburg, Germany — [3]Univ. Southampton, UK — [4]Univ. Hamburg, Germany — [5]Imperial College London, UK

We describe the Python-based user environment "Ubermag" to help scientists use well-established (micromagnetic) simulation packages.

Within Ubermag [1], researchers can express the physics problem they want to simulate in a scientist-friendly but machine readable problem definition based on Python syntax [2]. Ubermag translates this problem into the configuration files needed for micromagnetic simulation packages such as OOMMF or mumax3. On completion of the simulation, the computed data is presented back to the user at the Python level. Ubermag is often used in Jupyter Notebooks, and supports rich media to provide figures and equations within the notebook.

We report on the motivation for Ubermag, the design and implementation process, and our experiences made both from the perspective of science users and from the research software engineers. We touch on a range of topics, including interface design, domain specific languages, testing, packaging, Jupyter, and reproducibility.

This work was supported by EPSRC UK Skyrmion Grant EP/N032128/1, and the European research projects OpenDreamKit (676541) and MaMMoS (101135546).

[1] DOI 10.1109/tmag.2021.3078896; [2] DOI 10.1063/1.4977225

BP 29.3 Thu 15:45 H44

OCTOPOS.jl: A Julia-based tool for synonymous codon optimization — Simon Christ[1], Jan-Hendrik Trösemeier[2], and •Sophia Rudorf[1] — [1]Institute of Cell Biology and Biophysics, Leibniz University Hannover, Germany — [2]independent researcher

OCTOPOS.jl is a research software designed to optimize synonymous mRNA sequences for improved heterologous gene expression in various host organisms. Combining a detailed mechanistic model of in-vivo protein synthesis with machine learning, OCTOPOS.jl predicts protein expression based on codon choice. Originally developed as a Java desktop application, the software has been reimplemented in the Julia programming language to enhance performance, modularity, and scalability. The new implementation serves as the foundation for a graphical user interface and a web application, accessible at https://octopos.cell.uni-hannover.de/. These updates improve accessibility and usability, broadening its appeal to both computational and experimental biologists. OCTOPOS.jl supports organism-specific genetic sequence engineering and detailed analysis of translation dynamics, thus providing a valuable resource for the synthetic biology and biotechnology communities.

BP 29.4 Thu 16:00 H44

Invert pattern forming systems with BayesFlow to bridge the gap from simulation to experimental observation — •Hans Olischläger — Interdisciplinary Center for Scientific Computing (IWR) — Heidelberg University

The description of experimental systems by complex spatial models, be it with (stochastic) partial differential equations, agent-based simulation or otherwise, is often the condensation of all the central scientific hypotheses regarding a particular object of study.

I argue, that making progress in this kind of modelling is currently hindered by the lack of a tool that enables solving the following inverse problem: Given an observation, determine all the model configurations that are able to produce it. In other words, what is the posterior probability of all model configurations given some (set of) experimental data.

Instead of just preaching that in theory a Bayesian treatment would be nice, I will then continue to present such a tool: amortized Bayesian inference (as implemented in the software package BayesFlow). I will give examples on the classical Gierer-Meinhardt pattern forming PDE and a biophysical model, the Min system, which is used by E. coli to control cell division.

I will also take a step back to give a broader picture of the newly available statistical methods that support complex spatial modelling and their limitations. The aim is to provide some guidance on what you can and cannot infer from your state-of-the-art scientific simulator given observations, and how to do it.

BP 29.5 Thu 16:15 H44

FAIR Data Management for Soft Matter Simulations using NOMAD — •Bernadette Mohr[1], Esma Boydas[1], Nathan Daelman[1], José M. Pizarro[1], Tristan Bereau[3], Claudia Draxl[1], Luca M. Ghiringhelli[4], Martin Girard[2], Denis Usvyat[6], Roser Valentí[7], Silvana Botti[5], and Joseph F. Rudzinski[1,2] — [1]CSMB, HU Berlin — [2]MPIP Mainz — [3]ITP, Heidelberg Uni. — [4]Dept. of Mater. Sci. and Eng., FAU Erlangen — [5]RC-FEMS and Faculty of Physics, RUB Bochum — [6]Inst. für Chem., HU Berlin — [7]ITP, GU FfM

NOMAD [nomad-lab.eu][1, 2] is an open-source, community-driven data infrastructure designed to facilitate FAIR data management in materials science. Currently, it supports over 60 computational codes and encompasses DFT, classical MD, and many-body methods. This contribution will focus on recent developments, following modern software practices, to enhance NOMAD's applicability to soft matter and biological systems, including support for coarse-grained representations and advanced workflows such as free energy calculations. Combined with a schema for representing force fields, molecular topologies, and hierarchical system structures, NOMAD tracks data provenance and streamlines data analysis and the creation of AI-ready datasets. The NOMAD framework meets the classical simulation community's needs for improved data management standards and provides a foundation for building a cohesive, interconnected scientific data ecosystem.

[1] Scheidgen, M. et al., JOSS 8, 5388 (2023).

[2] Scheffler, M. et al., Nature 604, 635-642 (2022).

BP 29.6 Thu 16:30 H44

Estimation of kinetic rates by constrained optimization — •Federico Marotta[1], Maria Zimmermann-Kogadeeva[1], Peer

Bork[1], Julia Mahamid[1], and Sophia Rudorf[2] — [1]European Molecular Biology Laboratory — [2]Leibniz Universität Hannover

Biological systems often rely on molecular motors to perform useful work. The kinetics of the reactions in a motor's cycle can be easily investigated *in vitro* or in model organisms, but it is difficult to generalize them to a different system. We present a method to estimate the transition kinetics in an uncharacterized system, where minimal data are available, by leveraging a reference system where the kinetics have been elucidated. The motor's activity is represented as a continuous-time Markov chain, characterized by an infinitesimal generator matrix Q whose entries are functions of the transition rates of the cycle (the vector ω) and possibly of the concentrations of external molecules. In the uncharacterized system, the available data induce a constraint on the admissible rates. By employing an extremum principle, we estimate the rates ω_{unc} that minimize the kinetic distance with respect to the reference rates ω_{ref} while respecting such constraint. As an application of this strategy, we describe a model of the translation elongation cycle, where reference data are available for *E. coli in vitro*, and estimate the rates either *in vivo* or in a different organism, under constraints on the total elongation time or the steady-state occupancies, respectively.

BP 29.7 Thu 16:45 H44

Software provisioning for HPC and RSE — •Martin Lang[1,2], Henning Glawe[1,2], Jehferson Mello[1,2], and Hans Fangohr[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Free-Electron Laser Science, Hamburg, Germany — [3]University of Southampton, Southampton, UK

All research software relies on existing libraries for various functionalities such as low-level math operations, FFTs, IO, or other domain-specific operations. Installing these dependencies, potentially based on different compilers or in multiple versions, with all inter-dependencies fulfilled is notoriously difficult.

In the first part of this talk we introduce the open-source package manager Spack, which has a strong focus on HPC and research software. Spack can install software in multiple versions and variants, and supports optimised compilation for the underlying hardware, including compiling on exotic hardware. It comes with a large, community-provided collection of commonly used packages. Spack's packaging files make it easy to specify required dependencies, provide optional features of a software, and ensure compatibility with other libraries.

In the second part we present the concrete setup at our institute. We use Spack to provide the software stack on the local HPC, including pre-compiled packages and toolchains (sets of compilers and libraries) for users to compile their own software. We report on requirements and challenges, and how we address these with Spack. We also touch on scripting the Spack-based installation process including the option to recreate the HPC software environment on a scientist's laptop.

BP 29.8 Thu 17:00 H44

Small scale Research Software Engineering — •Simon Christ — Leibniz Universität Hannover, Institut für Zellbiologie und Biophysik, Computational Biology

While we are in dire need of research software organizations on a faculty level or larger, small scale software engineering, that is one research software engineer in a group or institute, is something that can be achieved in a short time frame and is probably the most common form today. A field report from Computational Biology where research software engineers are involved in modeling, developing solutions, teaching and maintenance.

BP 29.9 Thu 17:15 H44

Estimation of pKa values in membrane bound proteins — •Jesse Jones[1], Nereu Montserrat i Busquets[1,2], Ana Gamiz Hernandez[3], Ville Kaila[3], and Maria Andrea Mroginski[1] — [1]Technische Universität Berlin, Berlin — [2]Freie Universität Berlin, Berlin — [3]Stockholm Universität, Stockholm

Many key bioenergetic processes involving electron and proton reactions take place in membrane bound protein complexes, generating a proton motive force. Yet the ionizable groups which facilitate these reactions are often buried in hydrophobic pockets in the membrane. These processes are mainly described through pK_a values, which continue to be poorly understood and difficult to obtain despite structural, biochemical and computational advances. Hence, estimating pK_a values of these residues without the need for weeks of work in a laboratory, is important to describe the dynamics of the system, providing information on possible proton pathways. In this work we preview Karlsberg3, a software which uses a Poisson Boltzmann Equation solver (APBS) for proteins and calculates pKa values. Karlsberg3 is, in contrast to its predecessor Karlsberg2+, parallelized, running in modern software environments, and able to take membranes into consideration.

BP 29.10 Thu 17:30 H44

The teachingRSE project - Towards a professionalization of RSE education. — •Florian Goth[1] and Simon Christ[2] — [1]Universität Würzburg, Institut für theoretische Physik und Astrophysik, Am Hubland, 97074 Würzburg — [2]Leibniz Universität Hannover, Institut für Zellbiologie und Biophysik, Herrenhäuser Str. 2 30419 Hannover

At the deRSE23, the second conference for research software engineering(RSE) in Germany, a group of people came together for a small workshop to discuss how to deal with questions revolving around RSE education. Overwhelmed by the immense resonance to that workshop we took home a tremendous amount of feedback that made obvious that a short blog post will not suffice to adequately represent it. Now it is two years later, and the project produced its first output, the second position paper https://arxiv.org/abs/2311.11457 of de-RSE e.V. and it has sprawled out into a multitude of follow-up projects. In this talk, I will give an overview over the original ideas that we tried to convey in the position paper, and go into more detail on how domain sciences like physics need to change in light of this new specialization.

BP 29.11 Thu 17:45 H44

Python-Based Analysis Pipeline for the Quantification of Mechanics in Neural Organoids — •Michael Frischmann[1,2], Elijah R. Shelton[1], Achim T. Brinkop[1,2], and Friedhelm Serwane[1,2,3] — [1]Faculty of Physics & Center for NanoScience, LMU Munich, Germany — [2]Institute of Biophysics, Ulm University, Ulm, Germany — [3]SyNergy & GSN, Munich, Germany

Neuronal tissues form under the influence of mechanical forces guiding cellular movements. In the mammalian retina, neuronal translocations occur over hours. However, mechanical probing at those timescales in situ have posed experimental challenges. We employed magnetic ferrofluid droplets in mouse stem cell-derived retinal organoids to probe tissue mechanics from seconds to hours. To quantify tissue strain we have developed a Python-based analysis pipeline featuring an accessible graphical user interface (GUI). This pipeline automates strain quantification, image segmentation, and fitting procedures, enabling high-fidelity creep compliance measurements over extended durations. Our measurements reveal power-law scaling of dynamic compliance as well as tensile loss and storage modulus, consistent with soft glassy rheology just above the glass transition. These results demonstrate that neuronal tissues remodel in a scale-free manner while maintaining solid-like properties. This discovery provides a framework for understanding how mechanical signals may govern connectivity in the central nervous system. Integrating neural organoid models, mechanical probing, and computational methods, prepares us to investigate the interplay between biomechanics and neurodevelopment.

BP 30: Protein Structure and Dynamics

Time: Thursday 15:00–18:00 Location: H46

BP 30.1 Thu 15:00 H46

A protein sensor for plasma membrane lipid composition – insights from coarse-grained simulations — Saara Lautala and •Sebastian Thallmair — Frankfurt Institute for Advanced Studies, Frankfurt a.M., Germany

Extended synaptotagmins (E-Syts) are tethering proteins, which keep the plasma membrane (PM) and the endoplasmic reticulum (ER) membrane in close proximity at ER-PM contact sites. C2 domains are responsible for the binding of E-Syts to the PM. After depletion of phosphatidylinositol 4,5-bisphosphate PI(4,5)P_2, resynthesis of PI(4,5)P_2 takes place at ER-PM contact sites and thus, requires their integrity. The terminal C2C domain of E-Syt3 is known to bind PI(4,5)P_2. This results in an apparent paradox as the membrane binding and thus the tethered ER-PM contact site potentially become instable upon PI(4,5)P_2 depletion.

Here, we applied coarse-grained molecular dynamics simulations with the Martini 3 force field to investigate the membrane binding of the E-Syt3 C2C domain. Our simulations show that the C2C domain not only exhibits a binding hotspot for PI(4,5)P_2, but an additional binding hotspot for phosphatidylserine (PS) as well as a region binding to the membrane core. We will discuss that binding to PS results in a reorientation of the protein on the membrane surface and compare the different binding strengths. Overall, the PS binding site not only contributes to the ER-PM contact site integrity upon PI(4,5)P_2 depletion, but might also play a role in sensing low PI(4,5)P_2 levels.

BP 30.2 Thu 15:15 H46

Cross correlations in the Fluctuation-Dissipation Relation Reveal Solvent Friction in Hydrophobic Folding Transition — •Niklas Wolf, Viktor Klippenstein, Madhusmita Tripathy, and Nico F. A. van der Vegt — TU Darmstadt, Darmstadt, Germany

The Generalized Langevin Equation is a powerful tool for modeling and understanding the conformational dynamics of molecules in solution. However, recent works[1] have demonstrated that for these kinds of applications, the usual fluctuation-dissipation relation connecting the statistics of the random force to the memory kernel could contain a cross-correlation term. This raises the question of how the memory kernel should be extracted from simulation data and if a naive approach via the Volterra equations even gives a kernel related to a Markovian friction coefficient. We propose an approximation[2] to account for the cross-correlation term and show in a systematic study[3] that this approximation leads to an improved description of long-time dynamics and transition rates. Finally, we show that cross-correlations play an important role in the coil-to-globule transition of a hydrophobic polymer under various solvent conditions, where a naive approach would predict a significant violation of the Stokes-Einstein relation and give a poor description of barrier crossing times with rate theories.

[1] H. Vroylandt 2022 EPL 140 62003

[2] V. Klippenstein N. F. A. van der Vegt 2021 J. Chem. Phys. 154 191102

[3] N. Wolf et al. J. Chem. Phys. (under Review)

BP 30.3 Thu 15:30 H46

Multiscale simulation of protein phase separation — •Supriyo Naskar, Kurt Kremer, and Oleksandra Kukharenko — Max Planck Institute for Polymer Research, 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 level coarse-grained modelling techniques with data-driven machine-learning methods to explore the structural differences and multidimensional energy landscape of ubiquitin and SUMO and their conjugates. We finally study 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 instructing further experiments through adjustment of relevant parameters.

BP 30.4 Thu 15:45 H46

Sequence specificity and polymer physics — •Martin Girard — Max-Planck Institute for Polymer Research, Mainz, Germany

Sequence properties of disordered proteins in the context of phase separation has led to development of molecular grammar. So far, this has led to the development of empirical parameters tied to protein sequences.

Using surrogate models for low-complexity sequences, I will show that sequence-property relations are tied to the polymer collapse transition. I will further discuss implications for biological systems.

Invited Talk BP 30.5 Thu 16:00 H46

Topology in biological matter - are there double knots in proteins or maybe even more complicated knots? Prediction and in vitro verification. — •Joanna I Sulkowska — University of Warsaw, Banacha 2C, 02-097, Poland

We have been aware of the existence of knotted proteins for over 30 years-but it is challenging to predict what is the most complicated not that can be formed in proteins. Recently, based on AlphaFold (AF) method we predicted new and the most complex knotted topologies recorded to date - double trefoil knots (see AlphaKnot database). We found five domain arrangements that result in a doubly knotted structure in almost a thousand proteins. The double knot topology is found in knotted membrane proteins from the CaCA family, that functions as ion transporters, in the group of carbonic anhydrases that catalyze the hydration of carbon dioxide, and in the proteins from the SPOUT superfamily that gathers 31 knotted methyltransferases with the active site-forming knot.

Herein, I will present the first crystal structure of a double knotted protein TrmD-Tm1570 from Calditerrivibrio nitroreducens from SPOUT superfamily. The protein consists of two domains TrmD and Tm1570, each embedding a single trefoil knot, which can function on their own. We show that it folds in vitro and is biologically active.

I will also explain how AF and AI methods can be used to design artificially knotted proteins that can be obtained in vitro. This shows that AF, while predicting structure, also takes into account folding and overcoming a non-trivial looping pathway.

15 min. break

BP 30.6 Thu 16:45 H46

Single molecule FRET studies on folding properties of multidomain protein fragments — •Alida Meyer[1], Alexandros Katranidis[2], Nuno Bustorff[2], and Jörg Fitter[1,2] — [1]RWTH Aachen University, I. Physikalisches Institut (IA), AG Biophysik, Aachen, Germany — [2]Forschungszentrum Jülich, ER-C-3 Structural Biology, Jülich, Germany

Protein folding and unfolding are crucial for cellular function and stability. This study emloys single-molecule Förster resonance energy transfer (smFRET) to investigate structural transitions in yeast phosphoglycerate kinase (yPGK). We focus on its two-domain structure and the relationship between the Rossmann-fold topology and folding intermediates. Earlier studies with full-length yPGK labelled with fluorescent dyes at multiple different positions allowed to map several different intra-molecular distances during unfolding transitions [1,2]. To mimic co-translational folding properties, we performed smFRET measurements with truncated yPGK fragments. The results are compared with those of full-length proteins, including whether the same type of unfolding transition occurs as in the full-length protein (e.g., two state transitions or compact intermediates). In addition, the results from truncated fragments are also compared with nascent-chain folding in ribosome-nascent chain complexes (RNCs), analyzed via cryo-electron microscopy. These methods provide insights into how domain topology and neighboring structural elements influence multidomain protein folding. [1] Cerminara et al., Biophysical Journal, 2020, 118, 688 [2] Bustorff et al., Biomolecules, 2023, 13, 1280

BP 30.7 Thu 17:00 H46

Probing the dynamics of small unilamellar vesicles inside Synapsin pools using X-ray photon correlation spectroscopy — •Titus Czajka[1], András Major[1], Hendrik Bruns[1], Christian Hoffmann[2], Dragomir Milovanovic[2], and Tim Salditt[1] —

[1]Georg-August-Universität Göttingen — [2]Deutsches Zentrum für Neurodegenerative Erkrankungen, Berlin

The dynamics of many subcellular biological processes are difficult to access directly with microscopic techniques due to the resolution limit. Length and time scales beyond those accessible by conventional light microscopy can be probed via X-ray photon correlation spectroscopy (XPCS), even in dense media, by analysing the intensity autocorrelation function at different scattering vectors. However, the low scattering cross section of dilute biological samples and the sensitivity to radiation damage complicate the application of XPCS to biological systems. We have coated silica nanoparticles with a lipid bilayer to improve the scattering strength and overcome these challenges. Using such colloid-supported lipid bilayers (CSLBs), we have studied the dynamics of small unilamellar vesicles within synapsin protein pools, a system that exhibits evidence of both liquid-like and network-like phases. Our results show distinct diffusion constants at varying protein concentrations and provide evidence for non-diffusive behaviour within the pools.

BP 30.8 Thu 17:15 H46

Novel sample delivery for small nanoparticles and biomolecules for cryo-em — •Kevin Janson[1], Armando D. Estillore[1], Jiri Wald[4,5,6], Madeline Memovich[1], Thomas Marlovits[4,5,6], Amit K. Samanta[1,3], and Jochen Küpper[1,2,3] — [1]Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Department of Physics, Universität Hamburg, Hamburg, Germany — [3]Center for Ultrafast Imaging, Universität Hamburg, Hamburg, Germany — [4]Centre for Structural Systems Biology, Hamburg, Germany — [5]Institute of Structural and Systems Biology, University Medical Centre Hamburg-Eppendorf, Hamburg, Germany — [6]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Cryo-electron microscopy (Cryo-EM) is one of the key techniques in the field of structural biology. Recent years brought considerable improvements both on the software and hardware of the microscopes, and resolving high-resolution structures of proteins has become a standard procedure. However, most cryo-EM grids are still prepared by plunge freezing, a technique developed about ~40 years ago. During this process, proteins can be exposed to the air-water interface, possibly causing a preferential orientation or damaging their structure. We present the novel freeze-and-deposit sample delivery approach to deposit particles for cryo-EM using cryogenic shockfreezing technology. The cooling process produces cold high-density beams of nanoparticles. In this process, nanoparticles and macromolecules are aerosolized and rapidly cooled in the gas phase using a cryogenic buffer-gas cell.

BP 30.9 Thu 17:30 H46

Laser flash melting restores native protein conformation after cryoEM preparation by soft-landing, native electrospray ion beam deposition. — Sarah V. Barrass[1], Tim K. Esser[2], Nathan J. Mowry[1], Lukas Eriksson[2], Jakub Hruby[1], Laurence Seeley[3], Marcel Drabbels[1], Lindsay Baker[3], •Stephan Rauschenbach[2], and Ulrich J. Lorenz[1] — [1]EPFL Lausanne — [2]Univ. of Oxford, Dept. of Chem.. — [3]Univ. of Oxford, Dept. of Biochem.

Electron cryo microscopy (cryoEM) is today the dominating method for protein structure determination. Samples for cryoEM consist of thin, freestanding layers of amorphous ice in which proteins are embedded. Conventionally, these samples are prepared by shock-freezing of thin water films held in grid holes.

Alternative sample preparation methods are being developed, as the plunge-freezing method is not compatible with all types of protein sample. One of these methods is electrospray ion beam deposition (ESIBD) where mass-selected proteins from the gas-phase are landed on a thin amorphous carbon film in vacuum and embedded in ice grown from the gas phase for imaging. Recently it was shown that this method yields atomically resolved protein structures characterised by small changes in ternary structure due to dehydration.

Here we show that the dehydration can be reversed by irradiating the sample with short laser pulses, effectively melting the ice for a short time, allowing the protein to recover the native conformation, before the ice rapidly re-vitrifies.

BP 30.10 Thu 17:45 H46

Native Electrospray Ion Beam Deposition for Atomic-level Structure Analysis of Membrane Protein — •Jingjin Fan, Tim Esser, Clare De'Ath, Lukas Eriksson, Abdul Aziz Qureshi, Abraham Abraham, Laurence Seeley, Lindsay Baker, Carol Robinson, and Stephan Rauschenbach — The Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford OX1 3QU, United Kingdom

Membrane proteins play vital roles in cellular physiology, but their structural analysis remains challenging due to heterogeneity, flexible conformations, and demanding native conditions. To address these challenges, we established electrospray ion beam deposition (ESIBD) to directly couple native mass spectrometry (MS) with cryogenic electron microscopy (cryo-EM) for studying membrane protein structures.

Standard membrane proteins, including aquaporin Z (AqpZ) and ammonium transporter B (AmtB), were selected as testing models. By optimizing surfactant, the ion transfer in vacuum and the embedding of the proteins after landing we successfully manipulated membrane protein particles and achieved soft-landing on grids, evidenced by high-resolution imaging in cryoEM.

Our results demonstrate that the membrane structures can be preserved even in the absence of visible micelle.This molecular-level structural analysis captured by ESIBD in vacuum provides new insights into the correct folding of membrane proteins and understanding fundamental questions in structural biology.

BP 31: Active Matter IV (joint session BP/CPP/DY)

Time: Friday 9:30–13:00 Location: H44

Invited Talk BP 31.1 Fri 9:30 H44

Wave propagation in systems of active filaments — •Kirsty Y. Wan — Living Systems Institute, University of Exeter, UK

Active hair-like protrusions called cilia are found in many eukaryotes where they produce physiological flows for a variety of functions. Cilia assume a myriad of configurations both external to an organism for the purposes of feeding or swimming motility, but also internally where they mediate mucociliary clearance in vertebrate tissues. Single cilia can propagate large-amplitude non-decaying bending waves, even in the absence of a cell body. These waves assume a variety of stereotyped forms and frequencies, depending on the species. Multiple cilia also interact to produce different types of local and global coordination patterns, including robust metachronal waves. Do these dynamic states of coordination arise spontaneously, or do they require some form of internal control by the cell or animal? We propose new and emerging organisms to address these questions.

BP 31.2 Fri 10:00 H44

Metabolic activity controls the emergence of coherent flows in microbial suspensions — •Florian Böhme[1], Alexandros Fragkopoulos[1,2], Nicole Drewes[2], and Oliver Bäumchen[1,2] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Photosynthetic microbes have evolved and successfully adapted to the spatio-temporal variations of environmental parameters within their habitat. In the abscence of light, they can still sustain their biological functionality and metabolic activity through aerobic respiration. However, for the soil-dwelling microalga *Chlamydomonas reinhardtii*, their environment may be deprived of both oxygen and light, resulting in a significant reduction of their swimming velocity [1]. Here, we study the effect of motility and cell density of *C. reinhardtii* in a confined system, on the emergence of bioconvection [2]. This collective phenomenon can be reversibly switched by light and arises due to the natural tendency of the bottom-heavy cells to move against gravity. We show that the rate at which the system evolves, as well as the dominant wavelength of the instability can both be directly controlled by the number density of cells. Further, we provide insights on the internal flow fields and density profiles of single bioconvection plumes for different parameters.

[1] A.A. Fragkopoulos et al., *J. R. Soc. Interface* **18**, 20210553 (2021).
[2] A.A. Fragkopoulos et al., *arXiv*:2407.09884 (2024)

BP 31.3 Fri 10:15 H44

Tumbling *E.coli* in bulk and close to surfaces — •Pierre Martin[1], Tapan Chandra Adhyapak[2], and Holger Stark[1] — [1]Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Indian institute of science education and research (IISER), Tirupati, India

Escherichia coli (*E. coli*) swims by rotating multiple flagella which are connected to the cell body forming a thick bundle. To change direction, *E. coli* performs tumble events by reversing the rotation of one or more flagella. The involved filaments undergo a series of polymorphic transformations, altering both their helicity and handedness. This complex phenomenon involves the interplay of semiflexible filaments and hydrodynamic flow fields.
Here, we have developed a detailed numerical framework to simulate *E. coli*, capturing the full dynamics of flexible flagella, including their polymorphism and their hydrodynamic interactions. The filaments and the cell body are embedded in a viscous fluid, which we model using multi-particle collision dynamics. We analyzed a large number of tumble events, with fixed tumble time or taken from a gamma distribution, exploring the roles of hook and flagellar flexibility as well as flagellar polymorphism. We find that they strongly influence the distribution of tumble angles. Finally, we also show that close to a flat surface the mean tumble angle is strongly shifted to smaller values. This indicates that tumble events may not be recognized, which could give the impression of suppressed tumbling near surfaces.

BP 31.4 Fri 10:30 H44

***Trypanosoma brucei* (un)chained - effects of confinement on a parasitic microswimmer** — •Hannes Wunderlich[1], Marinus Thein[2], Lucas Brehm[2], Klaus Ersfeld[2], and Matthias Weiss[1] — [1]Experimental Physics I, University of Bayreuth — [2]Laboratory of Molecular Parasitology, University of Bayreuth

Trypanosoma brucei is a parasitic unicellular microswimmer that causes the African sleeping sickness. An active spiral movement of the parasite, mediated by a microtubule-driven flagellum that wraps around the cell body, is mandatory to evade the host's immune system while exploring tissues and blood vessels. In addition, the nematic subpellicular micotubule array plays a pivotal role in the elasticity, propulsion, and navigation of the parasite. To study the features and mechanisms behind the cell's motion in such complex environments, we have mimicked spatial confinement in microfluidic devices with different geometries. Our data show that spatial constraints in narrow channels and channel networks can improve cell locomotion of wild-type trypanosomes, supposedly due to the interaction of the elastic cell body and nearby walls. The addition of microtubule-disrupting drugs or the use of mutant strains with altered post-translational modifications of microtubules resulted in significantly altered swimming velocities and marked changes in the intermittent switching between run and tumble phases. Shape analyses of individual cells suggest that microtubules in the sub-pellicular array, the corset that keeps trypanosomes in their native spindle-like shape, are most affected in these cases.

BP 31.5 Fri 10:45 H44

Micro-swimmer motility in presence of signaling factors — Agniva Datta, Robert Grossmann, and •Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Germany

The navigation of bacteria through aqueous environments, driven by the rotation of helical flagella, has been a significant region of interest in the biophysics community for the last few decades. In this study, we focus on the motility of our model organism, Pseudomonas putida, which exhibits persistent mobile episodes (Active Brownian motion) interrupted by stochastic reorientation events (turns), driven by flagellar self-propulsion, thereby leading to a run-and-turn motility.

Key motility parameters including tumbling rates, run lengths, trajectory persistence (rotational diffusion coefficient), and the characteristics of the self-propulsion force*are hypothesized to depend on the density of quorum-sensing autoinducer molecules, produced by the bacteria themselves as signaling factors. To test this hypothesis, we expose swimming bacteria to aqueous environments with controlled autoinducer concentrations and analyze the resulting changes in motility patterns. Through a combination of experimental data and theoretical modeling, we aim to elucidate the principles of micro-swimmer motility in presence of signaling molecules.

BP 31.6 Fri 11:00 H44

Collective dynamics of active dumbbells near a circular obstacle — •Chandranshu Tiwari[1] and Sunil Singh[2] — [1]Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India. — [2]Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India.

We present the collective dynamics of active dumbbells in the presence of a static circular obstacle using Brownian dynamics simulation. The active dumbbells aggregate on the surface of a circular obstacle beyond a critical radius, and the aggregate size increases with the activity and the curvature radius. The dense aggregate of active dumbbells displays persistent rotational motion with a certain angular speed, which linearly increases with activity. Furthermore, we show a strong polar ordering of the active dumbbells within the aggregate. The polar ordering exhibits long-range correlation, with the correlation length corresponding to the aggregate size. Additionally, we show that the residence time of an active dumbbell on the obstacle surface increases rapidly with area fraction due to many-body interactions that lead to a slowdown of the rotational diffusion. This article further considers the dynamical behavior of a tracer particle in the solution of active dumbbells. Interestingly, the speed of the passive tracer particle displays a crossover from monotonically decreasing to increasing with the size of the tracer particle upon increasing the dumbbells' speed. Furthermore, the effective diffusion of the tracer particle displays non-monotonic behavior with the area fraction; the initial increase in diffusivity is followed by a decrease for a larger area fraction.

BP 31.7 Fri 11:15 H44

Free growth under tension — •Chenyun Yao and Jens Elgeti — Forschungszentrum Jülich GmbH, Jülich, Germany

Ever since the ground breaking work of Trepat et al. in 2009, we know that cell colonies growing on a substrate can be under tensile mechanical stress. The origin of tension has so far been attributed to cellular motility forces being oriented outward of the colony. Works in the field mainly revolve around how this orientation of the forces can be explained, ranging from velocity alignment, self-sorting due to self-propulsion, to kenotaxis.

In this work, we demonstrate that tension in growing colonies can also be explained without cellular motility forces! Using a combination of well established tissue growth simulation technique and analytical modelling, we show how tension can arise as a consequence of simple mechanics of growing tissues. Combining these models with a minimalistic motility model shows how colonies can expand while under even larger tension. Furthermore, our results and analytical models provide novel analysis procedures to identify the underlying mechanics.

15 min. break

BP 31.8 Fri 11:45 H44

A route to active turbulence in circular activity spots — •Arghavan Partovifard and Holger Stark — Institute of Theoretical Physics, Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623Berlin, Germany.

Active nematics exhibit distinctive behavior such as active turbulence and regular flow patterns under spatially varying activity [1]. Utilizing the Doi-Edwards theory supplemented by an active stress tensor [1], we investigate active nematics confined to a circular spot by switching off activity outside the spot. The open boundary allows topological defects to enter and leave the spot.

We calculate the total topological defect charge inside the spot using three approaches: counting all defects, measuring the rotation of the director field along the rim of the spot, and integrating the diffusive charge density. All methods agree that for spot radii just larger than the nematic coherence length, the system has a total topological charge of +1, where two +1/2 defects perform a regular swirling motion. As the radius increases, more defects enter and their motion becomes more and more chaotic. Ultimately, the charge per unit area saturates at the value characteristic of bulk active turbulence. For the range of radii where the total charge in the spot is +1, the nematic director exhibits shear-induced anchoring at an angle of 45° with respect to the tangent at the spot rim. With increasing radius, when more defects enter, the anchoring angle deviates from 45° but its distribution still peaks around this value.

[1] A. Partovifard *et. al.*, Soft Matter **20**, 1800 (2024)

BP 31.9 Fri 12:00 H44

Cognitive flocks: order-disorder transitions and threat evasion — •Priyanka Iyer[1], Cecilia Soroco[2], and Gerhard Gompper[1] — [1]Forschungszentrum Jülich — [2]University of British Columbia, Canada

Directed self-propulsion is ubiquitous in living organisms. From E.Coli dispersing in biofilms to migrating bird flocks, living organisms are constantly out-of equilibrium. By sensing their environment and adjusting their movement, organisms can exhibit emergent patterns and collective behaviors, such as self-organization in human crowds [1], bird flocks, and fish schools. The Inertial Spin Model (ISM) was introduced to explain the fast and robust propagation of information in bird flocks [2], when only alignment interactions are considered. However, more generally, agents exhibit a variety of interactions like local avoidance, cohesion and threat evasion. We show how such behaviors can be incorporated within the framework of the ISM. It is found that local avoidance introduces emergent noise in the system, triggering an order-disorder transition. Exploring the flock dynamics near this transition reveals a complex interplay between cohesion, alignment, and local avoidance, resulting in diverse behaviors such as pronounced shape and density fluctuations, and diffusive motion of the flock. Lastly, by applying the model to a stationary threat scenario, we analyze flock properties that govern threat information propagation in the flock.

[1] Iyer, P. et al. , Comm. Phys. 7.1 (2024): 379.
[2] Attanasi, A. et al. , Nat. Phys. 10, 691-696, (2014)

BP 31.10 Fri 12:15 H44

Myosin-independent amoeboid cell motility — •Winfried Schmidt, Alexander Farutin, and Chaouqi Misbah — Univ. Grenoble Alpes, CNRS, LIPhy, F-38000 Grenoble, France

Mammalian cell motility is essential for many physiological and pathological processes, such as the immune system, embryonic development, wound healing, and cancer metastasis. Cells have developed the amoeboid migration mode which allows them to move rapidly in a variety of different environments, including two-dimensional confinement, three-dimensional matrix, and bulk fluids. We introduce a model for an amoeboid cell where the cortex is described as a thin shell along the cell surface. The cell shape evolves due to polymerization of actin filaments and the forces acting on the cortex. We find analytically and numerically that the state of a resting, non-polarized cell can become unstable for sufficiently large actin polymerization velocities, resulting in the spontaneous onset of cell polarity, migration, and dynamical shape changes. Notably, this transition only relies on actin polymerization and does not necessitate molecular motors, such as myosin. These findings yield a deeper understanding of the fundamental mechanisms of cell movement and simultaneously provide a simple mechanism for cell motility in diverse configurations.

BP 31.11 Fri 12:30 H44

Active membrane deformations of a synthetic cell-mimicking system — Alfredo Sciortino[1], •Dmitry Fedosov[2], Gerhard Gompper[2], and Andreas Bausch[1] — [1]Physik Department, Technische Universität München, Garching bei München, Germany — [2]Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany

Biological cells are fascinating micromachines capable of adapting their shape due to the complex interaction between a deformable membrane and the dynamic activity of the cytoskeleton. We investigate the behavior of an active synthetic cell-mimicking system using simulations and experiments. In simulations, the model consists of a fluid vesicle with a few encapsulated growing filaments. In experiments, giant vesicles contain an active cytoskeletal network composed of microtubules, crosslinkers, and molecular motors. These active vesicles show strong shape fluctuations reminiscent of shape changes of biological cells. We analyze membrane fluctuations and show how the intricate coupling between soft confinement and internal active forces results in fluctuation spectra with distinct spatial and temporal scales, differing significantly from those of passive vesicles. Simulations demonstrate the universality of this behavior, quantifying the impact of correlated activity on the dynamics of membrane deformations. This model makes a step toward quantitative description of shape-morphing artificial and living systems.

BP 31.12 Fri 12:45 H44

Force Generation by Enhanced Diffusion in Enzyme-Loaded Vesicles — Eike Eberhard, •Ludwig Burger, Cesar Pastrana, Giovanni Giunta, and Ulrich Gerland — Physik komplexer Biosysteme, Technische Universität München, Deutschland

Recent experiments show that the diffusion coefficient of some metabolic enzymes increases with the concentration of their cognate substrate, a phenomenon known as enhanced diffusion. In the presence of substrate gradients, enhanced diffusion induces enzymatic drift, resulting in a non-homogeneous enzyme distribution. In this work, we study the behavior of enzyme-loaded vesicles exposed to external substrate gradients using a combination of computer simulations and analytical modeling. We observe that the spatially inhomogeneous enzyme profiles generated by enhanced diffusion result in a pressure gradient across the vesicle, which leads to macroscopically observable effects, such as deformation and self-propulsion of the vesicle. Our analytical model allows us to characterize dependence of the velocity of propulsion on experimentally tunable parameters. The effects predicted by our work provide an avenue for further validation of enhanced diffusion, and might be leveraged for the design of novel synthetic cargo transporters, such as targeted drug delivery systems.

BP 32: Computational Biophysics II

Time: Friday 9:30–13:00 Location: H46

BP 32.1 Fri 9:30 H46

From slabs to cubes: finite size effects in biomolecular simulations — •Rodrigo F. Dillenburg and Martin Girard — Max Planck Institute for Polymer Research, Mainz, Germany

Coarse-grained simulations of intrinsically disordered proteins have become essential to the study of biomolecular condensates. Multiple choices of force fields, simulations techniques and box geometries have been employed in such studies, assuming that results will converge due to the law of large numbers. This assumption is, however, not automatically valid for all systems and needs to be carefully examined to assure the validity of the results. In our work we focused on the choice of box geometry (cubic or slab) and statistical ensemble (canonical or grand-canonical) and its effect on the phase behavior of systems undergoing liquid-liquid phase separation. Our results allow us to estimate if a system can be approximated by the thermodynamic limit or if finite size effects have to be taken into consideration. We are able to derive expressions for these corrections depending on the choice of system and are also able to relate it to condensate properties such as surface tension. Our results provide a rational approach to selecting the most appropriate simulation methods for a given system.

BP 32.2 Fri 9:45 H46

Interactions of Imidazolium with Elastin-Like Polypeptides: A Molecular Dynamics Study — •Julia Keil and Nico F. A. van der Vegt — Technische Universität Darmstadt, Germany

Biological buffers are commonly used to adjust the pH value of protein solutions and are typically assumed not to affect other properties of the system.[1] However, a series of experimental observations suggest buffer-specific effects on protein stability.[2] Despite these findings, studies on these effects remain limited, and the underlying mechanisms are still poorly understood.[2-4]

We performed molecular dynamics simulations at constant pH[4] to investigate the interactions between the buffer imidazolium (IMI) and elastin-like polypeptides (ELPs) that contain chemically different amino acids at their variable positions. Our analyses revealed a local accumulation of imidazole (IMI^{o}) around the ELPs and its hydrogen bonding to the ELP backbone, regardless of the ELP composition. In contrast, interactions with imidazolium (IMI^{+}) were found to depend on the ELP composition. A strong local accumulation of IMI^{+} was observed around ELPs containing negatively charged groups, accompanied by hydrogen bonding to their side chains. Conversely, local depletion of IMI^{+} occurred around ELPs with positively charged groups. As a result, the interactions of ELPs with IMI are determined by the specific composition of the ELPs.

[1] *Nat. Chem.* 2021, 13, 1023-1024 [2] *Curr. Opin. Colloid Interface Sci.* 2016, 23, 1-9 [3] *J. Pharm. Sci.* 2017, 106, 3, 713-733 [4] *J.*

Chem. Theory Comput. 2022, 18, 10, 6148-6160

BP 32.3 Fri 10:00 H46

Graphite-based Bio-mimetic Nanopores for Protein Sequencing and Beyond — •Chandan K. Das and Maria Fyta — Computational Biotechnology, RWTH Aachen University, Aachen, Germany

Protein sequencing via nanopores offers a transformative approach to bioanalytics, but challenges remain, particularly in linearizing unfolded proteins and controlling translocation speed through solid-state nanopores. This study introduces a novel solution: biomimetic graphite-based nanopores designed with nanometer-sized pores featuring a constriction zone inspired by the alpha-hemolysin protein pore. All-atom molecular dynamics simulations demonstrate the nanopores' ability to achieve ion selectivity and generate electro-osmotic flow (EOF) within the pore lumen due to tailored surface charges. This innovation enables the detection of peptides at the single amino acid level by analyzing ionic current fluctuations during peptide translocation. A critical feature of this design is its capacity to balance hydrodynamic drag, induced by EOF, with electrophoretic force (EPF), facilitating peptide linearization and extending amino acid residence time within the constriction zone. These advancements significantly enhance sequencing resolution and accuracy. Beyond protein sequencing, this technology holds potential for diverse applications, including seawater desalination via electrodialysis and renewable energy generation through salinity gradient-driven ion separation. By providing a robust computational foundation, this study advances the development of graphite-based biomimetic nanopores, offering versatile solutions for bio/nanotechnological challenges and sustainable energy innovations.

BP 32.4 Fri 10:15 H46

Helical transition of protein chain: An in silico study — •tika ram bhandari and martin girard — Max Planck Institute for Polymer Research, Mainz, Germany

Structural transformations in biomolecular systems are critical for physiological functions, with folding and unfolding transitions governing numerous cellular activities. Misfolding of proteins, however, is a key factor in the onset of severe diseases, emphasizing the need for comprehensive studies to understand and control these processes. Computational simulations provide valuable insights into such mechanisms. Here, we employed coarse-grained molecular simulations coupled with Hamiltonian Replica Exchange method to investigate the disordered-to-helical transition of IM30, the bacterial counterpart of the ESCRT-III. By systematically varying the strength of hydrogen bonds, we simulated an in-silico denaturation process, enabling a detailed analysis of the structural properties underlying this transition. Furthermore, we explore the impact of point mutations on the protein's helical propensity using free energy calculations. These approaches provide a deeper understanding of the molecular mechanisms influencing folding behavior and highlights the role of specific mutations in modulating protein structure.

BP 32.5 Fri 10:30 H46

Towards modeling cellular environments from cryo-electron tomography by high-confidence 3D template matching — •Sergio Cruz-León, Jan Philipp Kreysing, Maziar Heidari, Beata Turoňová, Martin Beck, and Gerhard Hummer — Max Planck Institute of Biophysics, Max-von-Laue-Str. 3, 60438, Frankfurt am Main, Germany

The simulation of biologically realistic systems requires precise knowledge of the composition and spatial arrangement of biomolecules in situ. This information can be obtained from cryo-electron tomography (cryoET), which images the interior of intact cells in 3D. However, feature identification is limited by the low signal-to-noise ratio and anisotropic resolution of the tomographic data. In this talk, I will present our recent advances in high-confidence 3D template matching (hcTM) for cryoET [1] and how we use hcTM to generate simulation-ready molecular models directly from cells [1,2]. hcTM enables the automated and comprehensive detection of a wide variety of macromolecular complexes within crowded eukaryotic cells. The high-confidence molecular assignments have driven both technical advances [3] and biological discoveries [1,2], fostering robust connections between molecular functionality, spatial localization, and cellular context. Thus, hcTM paves the way for modeling and simulating the dynamics of biomolecules in their native environment.

[1] Cruz-León, et al., Nat. Comm., 2024 [2] Kreysing*, Heidari*, Zila*, et al., BioRxiv, 2024 [3] Tuijtel, et al., Sci. Adv., 2024

BP 32.6 Fri 10:45 H46

Membrane insertion and channel formation of alpha-latrotoxins — •Andreas Heuer[1], Azadeh Alavizargar[1], Björn U. Klink[2,3], and Cristos Gatsogiannis[2,3] — [1]Institute for Physical Chemistry, University of Münster, Germany — [2]Center for Soft Nanoscience (SoN), University of Münster — [3]Institute for Medical Physics and Biophysics

Latrotoxins are the main toxic component of the venom of black widow spiders. It is known that the they provide ion channels in the plasma membrane, allowing, e.g., for a strong influx of Ca2+ ions which may induce a burst of neurotransmitters. Despite its importance, microscopic information about the microscopic structure of latroxin pore formation remained elusive.

In this presentation it is shown how detailed information can be gained by a combination of cryoEM, AlphaFold and Molecular Dynamics (MD) simulations [1]. From this analysis we can identify a unique mechanism of membrane insertion and channel formation for the example of Na+ and Ca2+ transport. From the MD simulations it is possible, e.g., to elucidate the efficiency and the time-scales of the transport processes and to show why the channel is efficient in transporting mono- and divalent ions but not trivalent ions.

[1] Klink, B.U., Alavizargar, A., Kalyankumar KS, Chen M, Heuer A, Gatsogiannis C (2024) Nature Communications 15, 8551

BP 32.7 Fri 11:00 H46

Understanding the impact of functionalized gold nanoparticles (AuNPs) on the lipid bilayer and interfacial water through atomistic molecular dynamics simulations — •Haifa Al Mamari, Srinivasa Varanasi, and Issam Ali — Sultan Qaboos University, Department of Physics

Functionalized gold nanoparticles (AuNPs) show promise as drug delivery systems due to their customizable size, shape, biocompatibility, and surface modifications. However, crossing cell membrane barriers is a challenge, requiring efficient penetration for effective drug delivery. Interfacial water and ions play a crucial role in the interaction between AuNPs and bilayers, making it essential to understand the structural and orientational effects on lipid bilayers. This study explores how nanoparticle surface charge and lipid chemistry impact AuNP-lipid bilayer interactions, focusing on anionic (carboxylate) and cationic (quaternary ammonium) AuNPs with zwitterionic (DPPC), anionic (DPPG), and cationic (DPTAP) bilayers using molecular dynamics simulations.Our analysis shows that AuNPs significantly alter bilayer properties, impacting the area per lipid, membrane thickness, acyl chain order, electrostatic potential, dipole alignment, and head and tail tilt angles. These changes enhance water dipole alignment and modify electrostatic potentials, depending on the nanoparticles surface charge. These insights emphasize AuNPs' potential to reshape membrane properties, providing valuable guidance for nanoparticle-based therapeutic development.

15 min. break

BP 32.8 Fri 11:30 H46

Swimming by spinning: spinning-top type rotations regularize sperm swimming into persistently progressive paths in 3D — •Xiaomeng Ren and Hermes Bloomfield-Gadêlha — School of Engineering Mathematics & Bristol Robotics Laboratory, University of Bristol, BS8 1UB Bristol, UK

Sperm swimming is essential for reproduction, with movement strategies adapted to specific environments. Sperm navigate by modulating the symmetry of their flagellar beating, but how they swim forward with asymmetrical beats remains unclear. Current methods lack the ability to robustly detect the flagellar symmetry state in free-swimming spermatozoa, despite its importance in understanding sperm motility. This study uses numerical simulations to investigate the fluid mechanics of sperm swimming with asymmetrical flagellar beats. Results show that sperm rotation regularizes the swimming motion, allowing persistently progressive swimming even with asymmetrical flagellar beats. Crucially, 3D sperm head orientation, rather than the swimming path, provides critical insight into the flagellar symmetry state. Sperm rotations during swimming closely resemble spinning-top dynamics, with sperm head precession driven by the helical beating of the flagellum. These results may prove essential in future studies on the role of symmetry in microorganisms and artificial swimmers, as body orientation detection has been largely overlooked in favor of swimming path analysis. Altogether, this rotational mechanism provides a reliable solution

for forward propulsion and navigation in nature, which would otherwise be challenging for flagella with broken symmetry.

BP 32.9 Fri 11:45 H46

Simulating Trypanosome Motility — •Florian Overberg, Gerhard Gompper, and Dmitry Fedosov — Theoretical Physics of Living Matter, Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

We investigate motility of the protozoan Trypanosoma brucei via numerical simulations, in which a trypanosome model is informed by experimental observations. The cell body is represented by a set of vertices distributed homogeneously on a pre-defined elongated surface, forming a triangulated elastic network of springs. This network model incorporates bending rigidity, area conservation, and volume conservation constraints. For the generation of propulsion, a flagellum is attached to the cell body. The flagellum consists of four parallel filaments, two of which are embedded in the body and used for generating a propagating bending wave. We examine the parasite behavior for various conditions, including different flagellum and body stiffnesses, beating frequencies, actuation wavelengths, and amplitudes. Our simulations yield swimming velocities and rotation frequencies around the swimming axis that are in a good agreement with experimental measurements. Additionally, we investigate the importance of various actuation characteristics, such as orientation of the beating plane and the stress-free conformation of the flagellum. We have also started to study parasite motility in a stationary blood suspension, which serves as a first step to understand trypanosome behavior in one of its natural environments such as blood vasculature.

BP 32.10 Fri 12:00 H46

Leveraging quantum data to advance machine-learning in (bio)molecular simulations — •Leonardo Medrano Sandonas[1], Mirela Puleva[2], Gianaurelio Cuniberti[1], and Alexandre Tkatchenko[2] — [1]TUD Dresden University of Technology, Germany. — [2]University of Luxembourg, Luxembourg.

The rapid advancement of machine learning (ML) applications in chemistry and physics has been driven by the increasing availability of comprehensive quantum-mechanical (QM) datasets. Recently, we introduced high-fidelity property data at the PBE0+MBD level of theory for both small [Sci. Data 8, 43, (2021)] and large [Sci. Data 11, 742, (2024)] drug-like molecules in equilibrium and non-equilibrium states. These datasets have been instrumental in advancing QM-based ML interatomic potentials [10.26434/chemrxiv-2024-bdfr0, (2024)] and enhancing semi-empirical (SE) methods [J. Phys. Chem. Lett., 11, 6835 (2020)], enabling accurate (bio)molecular simulations. In this presentation, we will discuss our recent efforts to improve the transferability and generalizability of the ML-corrected density functional tight-binding method. We demonstrate that equivariant neural networks significantly enhance the accuracy and scalability of ML-based many-body repulsive potentials trained on energies and forces of small organic systems. This approach facilitates the investigation of the energetic and structural properties of large drug-like molecules and molecular dimers. Hence, our findings indicate that combining ML with SE methods achieves both high accuracy and computational efficiency, paving the way for diverse applications in (bio)molecular simulations.

BP 32.11 Fri 12:15 H46

Calibrating 1D-0D Coupled Blood Flow Models: the potential of Neural Network based Surrogates — •Benedikt Hoock[1,2] and Tobias Köppl[3] — [1]Technische Universität München, School of Computation, Information and Technology — [2]Support by Computing Facilities of Leibniz-Rechenzentrum München — [3]Fraunhofer-Institut FOKUS, Berlin

Hydrodynamic models of the human arterial network can simulate the blood flow in parts or the whole body. The calculations can be simplified by solving the incompressible one-dimensional Navier-Stokes equations only for a set of larger vessels and coupling those at their outlets to a Windkessel model (*1D-0D approach*). Here, the right parametrization of the Windkessel parameters, i.e., the resistances and capacities, is crucial to obtaining realistic simulations. This can be done by calibrating the model parameters to match the model predictions with in-vivo blood pressure measurements. Since this requires many computationally expensive model evaluations, we test the potential of surrogates based on neural networks (NN). Once set up in an appropriate architecture, already ordinary fully connected NNs of moderate depth and width two can reproduce the simulations with high accuracy, advancing over e. g. the PINN approach due to their better trainability. We use these in an optimization algorithm to identify the target resistance and capacity with high precision in several test cases. Our efficient calibration scheme is an essential building block for an instantaneous visualization of the organ perfusion in a digital twin of a patient under different motion conditions on a digital treadmill.

BP 32.12 Fri 12:30 H46

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

The integration of machine learning (ML) and computational chemistry enables efficient prediction of quantum properties for complex molecules, crucial for advancing drug discovery and materials science. Our ML platform leverages Graph Convolutional Neural Networks (GCNNs) and the "sliding window" methodology to predict quantum mechanical parameters like partial atomic charges, overcoming traditional ab initio constraints. This approach scales to larger, biologically relevant molecules, enhancing molecular dynamics simulations and rational drug design.

Focusing on marine saponins -complex thalassochemicals with unique sulfated glycoside structures- our platform improves charge distribution predictions, enabling precise simulations of bioactive interactions. These advances highlight the therapeutic potential of marine saponins in oncology, lipid metabolism, and immune modulation. By applying our platform to marine saponins, this research bridges computational and experimental workflows, fostering the discovery of novel thalassochemicals for applications in functional foods, pharmaceuticals, and sustainability.

BP 32.13 Fri 12:45 H46

Ab-initio optimization and AI-powered inference for parametrizing complex biological models under low data availability — •Thomas R. Sokolowski — Frankfurt Institute for Advanced Studies (FIAS), Ruth-Moufang-Str. 1, 60438 Frankfurt am Main, Germany

Early development unfolds under diverse circumstances and time scales, but always facing the impacts of inevitable biological noise. To cope with this, various developmental mechanisms evolved, with their differences shaped by physical and environmental constraints. In spite of decades of research, we still lack theories that explain these processes truly mechanistically. Increasing computational power allows for constructing developmental models with increasing complexity, but since corresponding experimental data is scarce, the parametrization of such models becomes a key problem itself. I will contrast two strategies for parametrizing biophysical models in development and beyond: optimization of normative theories, and Bayesian inference. I will present a framework that unifies both strategies in a mathematically rigorous fashion and enables quantitative transition between them. I will then present our results combining both strategies for understanding embryogenesis in two organisms: (1.) optimization of a spatial-stochastic model of the gap gene system in Drosophila, and (2.) elucidation of robust cell-fate assignment in early mouse embryogenesis via AI-powered simulation-based inference (SBI). Our results highlight distinct developmental strategies that emerged under the different circumstances faced by the two organisms.

BP 33: Focus Session Chemical Imaging for the Elucidation of Molecular Structure II (joint session O/BP)

Unravelling the multiscale molecular heterogeneity at interfaces is one of the main challenges in modern biophysics and surface science due to the major role specific structural properties play in determining their macroscopic function and behavior. In the last few decades, several specialized chemical imaging techniques have been developed that can reveal many of these crucial structural details, representing an enormous advance in our elucidative capabilities. Clear examples of this range from super-resolution and 3D tomography to tag-free characterization down to the single-molecule level. This focus session will explore the vast range of methods and possibilities for characterizing the different structural aspects in heterogeneous molecular systems and specifically highlight the potential complementarity of the different techniques through multi-modal approaches. Overall, by bringing together different communities, this session aims to foster scientific exchanges that could spark the next major developments in chemical imaging.

Organized by
Martin Thämer (FHI Berlin), Alexander Fellows (FHI Berlin), and Kerstin Blank (University Linz)

Time: Friday 10:30–12:45 Location: H24

Invited Talk BP 33.1 Fri 10:30 H24

Multidimensional Super-resolution Imaging: Wasting Light to Learn New Things — •Steven Lee — University of Cambridge

The talk will outline two single-molecule fluorescence approaches that can be used to determine orthogonal metrics about a single emitter.

The first half introduces "POLCAM," a simplified single-molecule orientation localization microscopy (SMOLM) method based on polarised detection using a polarisation camera. POLCAM's fast algorithm operates over 1000 times faster than the current state-of-the-art, allowing near-instant determination of molecular anisotropy. To aid adoption, open-source image analysis software and visualization tools were developed. POLCAM's potential was demonstrated in studying alpha-synuclein fibrils and the actin cytoskeleton of mammalian cells. (Nature Methods 2024). The second approach focuses on "Single-Molecule Light Field Microscopy" (SMLFM), encoding 3D positions into 2D images for volumetric super-resolution microscopy. SMLFM shows an order-of-magnitude speed improvement over other 3D PSFs, resolving overlapping emitters through parallax. Experimental results reveal high accuracy and sensitivity in point detection, enabling whole-cell imaging of single membrane proteins in live primary B cells and high-density volumetric imaging in dense cytosolic tubulin datasets. (Nature Comms 2024)

Invited Talk BP 33.2 Fri 11:00 H24

MALDI mass spectrometry imaging: application examples ranging from food analysis to pharmaceutical research — •Andreas Römpp — Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany

Mass spectrometry imaging is an analytical technique that provides spatially-resolved molecular information for a wide range of compound classes. In contrast to many histological methods, it does not require labeling. The capabilities and limitations of MS imaging will be discussed on the basis of several application areas with a focus on food analysis and pharmaceutical research. In our study 'MALDI mass spectrometry imaging: from constituents in fresh food to ingredients, contaminants and additives in processed food' (https://doi.org/10.1016/j.foodchem.2022.132529) we analyzed a range of plant-based and meat-based food. The analysis of natamycin in cheese and acrylamide in gingerbread constitute the first mass spectrometry imaging measurements of a food additive and a food contaminant, respectively. MS imaging is the only method that can analyze the distribution of drug compounds in animal models or human tissue (without labeling). This is exemplified on the detection of anti-tuberculosis drugs in mouse model tissue including our most recent study on the clinical stage antibiotic BTZ-043 which has just been accepted for publication in Nature Communications (https://doi.org/10.1038/s41467-025-56146-9).

BP 33.3 Fri 11:30 H24

On-Surface Synthesis and Characterization of a Nitrogen-Containing Heterocycle — •Marco Thaler[1], Ricardo Ruvalcaba Briones[2], Matthias Zeilerbauer[1], Shadi Fatayer[2], and Laerte Patera[1] — [1]University of Innsbruck, Austria — [2]King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Nitrogen-containing heterocycles are fundamental building blocks in nature, forming the core of essential biomolecules and pharmaceuticals. This study demonstrates the on-surface formation of an N-heterocyclic organic compound via thermal activation of a tailored precursor. High-resolution non-contact atomic force microscopy (nc-AFM) provides bond-level resolution of the synthesized structures. Complementary scanning tunneling spectroscopy visualizes changes in the electronic structure resulting from the formation of the heterocycle. Density functional theory calculations (DFT) reveal the most probable reaction mechanism, highlighting the critical role of hydrogen release as the driving force of the reaction. These findings emphasize the versatility of on-surface synthesis as a powerful tool for creating complex organic compounds.

BP 33.4 Fri 11:45 H24

Elasticity Mapping of Nonahelicene with Submolecular Resolution by NC-AFM — •Max Halbauer[1], Takashi Kumagai[2], Martin Wolf[1], and Akitoshi Shiotari[1] — [1]Fritz-Haber-Institute, Faradayweg 4-6, 14195 Berlin, Germany — [2]Institute for Molecular Science, 38 NishigoNaka, Myo-daiji, Okazaki 444-8585, Japan

Controlled modification of atomic configurations of molecules and materials is an exciting goal for non-contact atomic force microscopy (NC-AFM). Certain changes like shifts of the electronic energy gaps may be expected, but are not well explored and not established on the molecular scale. Here we report quantitative measurement of atomic-scale deformation in single molecules with NC-AFM. Individual molecules of nonahelicene ([9]H) and coronene (Cor) were studied on a Ag(110) surface under ultrahigh vacuum and cryogenic conditions by the measurement of frequency-shift distance curves for this. The molecular responses can be replicated with an empirical Lennard-Jones model, but for [9]H an elastic contribution is required to account for its elastic nature. Furthermore, a 3D-force mapping technique, termed molecular deformation mapping (MDM), allows to study the lateral position dependence of the elastic response. The MDM of [9]H reveals a spatially strongly anisotropic behaviour for the elasticity, interaction forces, elongation and binding energy of the tip to the molecule. The result is rationalized in terms of an aromaticity model.

BP 33.5 Fri 12:00 H24

Detection and control of quantum proton ordering in hydrogen bonds at the atomic scale — •Yiqi Zhang — Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Directly probing the spatial arrangements and quantum nature of protons in hydrogen-bonded (H-bonded) materials and biosystems is the key to understand their macroscopic properties and functions. Here, exploiting bond-resolved atomic force spectroscopy (BR-AFS) combined with path-integral molecular dynamics method, we demonstrate for the first time that BR-AFS measurements along the apparent H-bond between proton donor and acceptor atoms allows the identification of both classical H-bonds with inherent directionality and non-classical H-bonds with quantum proton delocalization in self-assembled imidazole derivatives on surfaces. Unlike the conventional unidirectional H-bonding in linear chains, chiral cyclic hexamers exhibit unique quantum proton ordering in their ground states, which contain a mix

of classical and non-classical H-bonds, breaking rotational symmetry. Furthermore, we show the capability to switch the quantum-proton-ordering state on and off by altering the adsorption registry coupled with a collective transfer of six protons within the cyclic H-bonds. These findings open new pathways for detecting and controlling complex proton orders and for engineering proton-based quantum states with atomic-level precision.

BP 33.6 Fri 12:15 H24

Imaging of the conformations of individual β-cyclodextrins with non-contact AFM — Marko Grabarics[1], •Benjamin Mallada[1,2,3], Shayan Edalatmanesh[2,3], Stephan Rauschenbach[1], Pavel Jelinek[2,3], and Bruno de la Torre[2] — [1]Kavli Institute for Nanoscience Discovery, University of Oxford, UK — [2]CATRIN, Palacký University Olomouc, CZ — [3]Institute of Physics, Czech Academy of Sciences, CZ

Glycans, biopolymers essential to biology and materials science, are highly complex due to their structural diversity, conformational flexibility, and numerous possible isomers. Conventional methods often struggle to resolve these structures with atomic precision, especially under solvent-free conditions. We employ nc-AFM under UHV to determine the atomic structure of β-cyclodextrin (β-CD), a cyclic glucose molecule.

Our results reveal the adsorption geometries, hydroxy group positions, and stabilizing hydrogen bonds on a Au(111) surface. The primary face forms a closed hydrogen-bond network, while the secondary face exhibits pairwise interactions between OH groups of the same glucose monomer. DFT calculations validate these findings, enabling precise structural assignment and capturing subtle conformational differences.

This work highlights nc-AFM's capability to overcome the limitations of conventional sequencing techniques and represents the first application of nc-AFM to glycans. Future integration with ion deposition techniques could extend its utility to more complex glycans.

BP 33.7 Fri 12:30 H24

Domain size effects in the spectra of micro-heterogeneous samples — •Thomas Mayerhöfer[1,2] and Jürgen Popp[1,2] — [1]Leibniz Institute of Photonic Technology (IPHT), Albert-Einstein-Str. 9, 07745 Jena, Germany — [2]Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University, Helmholtzweg 4, 07743 Jena, Germany

Samples are often not composed of a single pure compound but are instead mixtures of different substances. Under the Bouguer-Beer-Lambert approximation, the absorbance spectra of such mixtures can be simply derived by summing the spectra of the individual components, with each spectrum weighted by the molar fraction of the corresponding compound.

In the context of wave optics, the resolving power of light at a given wavelength becomes crucial. If a microscope using light at this wavelength can distinguish structural details within the sample, the sample is classified as micro-heterogeneous. In this case, spatial averaging occurs at the intensity level, involving reflectance and transmittance rather than absorbance.

The shift from micro-heterogeneity to macro-heterogeneity is gradual and cannot be described by an analytical formula due to the wave nature of light. This has significant implications for spectrum interpretation, as it can lead to substantial variations in peak shapes, positions, and intensities, e.g., during mitosis.

BP 34: Statistical Physics in Biological Systems II (joint session DY/BP)

Time: Friday 11:30–13:00 Location: H43

Invited Talk BP 34.1 Fri 11:30 H43

Equilibrium and non-equilibrium dynamics of biological systems with memory — •Roland Netz — Freie Universität Berlin, Fachbereich Physik, Berlin

Biological systems are many-body systems. Thus, their dynamics, when described in terms of a low-dimensional reaction coordinate, is governed by the generalized Langevin equation (GLE), an integro-differential equation of motion which contains friction memory [1]. Two examples will be discussed:

Protein-folding kinetics is standardly described as Markovian (i.e., memoryless) diffusion in a one-dimensional free-energy landscape. By analysis of molecular-dynamics simulation trajectories of fast-folding proteins the friction is demonstrated to exhibit significant memory with a decay time of the same order as the folding and unfolding times [2,3,4]. Memory friction leads to anomalous and drastically modified protein kinetics: the folding and unfolding times are not dominated by free-energy barriers but rather by non-Markovian friction.

Active motion of organisms obviously is far from equilibrium. The parameters of an appropriate non-equilibrium GLE are extracted from trajectories. It is demonstrated that the motion of single-cellular algae is characterized by pronounced memory friction, which allows to classify and sort individual cells.

[1] Memory and Friction: From the Nanoscale to the Macroscale, BA Dalton, A Klimek, H Kiefer, F N Brünig, H Colinet, L Tepper, A Abbasi, RR Netz, https://arxiv.org/pdf/2410.22588

BP 34.2 Fri 12:00 H43

Mean transient drift of synaptic weights in feed-forward spiking neural networks with spike-timing-dependent plasticity — •Jakob Stubenrauch and Benjamin Lindner — BCCN Berlin and Physics Department HU Berlin, Germany

Spike-timing dependent plasticity (STDP) [1] is a phenomenological model for the dynamics of single synaptic weights. This concise microscopic (single-synapse) description allows for the derivation of macroscopic network theories, capturing for instance learning, forgetting, and representational drift.

For the development of such theories it is important to characterize the stochastic process of synaptic weights. Early attempts capture this process for Poissonian presynaptic spikes and conditionally Poissonian postsynaptic spikes [2]. However, since STDP depends on fine spike-timing differences below 20 ms [1], it is important to characterize the synaptic dynamics for neuron models that describe the fast response mechanistically.

Leveraging a recent theory [3] as well as established results for the leaky integrate-and-fire neuron [4,5], we analytically compute the drift and diffusion of feed-forward synapses in a setup where a layer of presynaptic Poisson processes feeds into a recurrent network of leaky integrate-and-fire neurons.

[1] Bi and Poo, J. Neurisci. (1998) [2] Kempter et al., Phys. Rev. E (1999) [3] Stubenrauch and Lindner, Phys. Rev. X (2024) [4] Brunel et al., Phys. Rev. Lett. (2001) [5] Lindner and Schimansky-Geier, Phys. Rev. Lett. (2001)

BP 34.3 Fri 12:15 H43

A Biophysical Model for Temperature-Sensitivity of Neurons — •Julian Voits[1], Wojciech Ambroziak[2,3], Jan Siemens[2,4], and Ulrich S. Schwarz[1,5] — [1]Institute for Theoretical Physics, University of Heidelberg, Germany — [2]Department of Pharmacology, University of Heidelberg, Germany — [3]Department of Translational Disease Understanding, Grünenthal GmbH, Aachen, Germany — [4]Molecular Medicine Partnership Unit (MMPU), European Molecular Biology Laboratory (EMBL), Heidelberg, Germany — [5]BioQuant-Center for Quantitative Biology, University of Heidelberg, Germany

Control of body temperature is essential for our well-being and especially important during periods of fever or heat acclimation, e.g. due to traveling or climate change. An essential element of body temperature control are temperature-sensitive neurons, particularly warm-sensitive ones in the preoptic area of the hypothalamus. Since the discovery of temperature-sensitive ion channels, it has become clear that the underlying molecular mechanisms are rather diverse. In this work, we introduce a mathematical model based on a reduced version of the Hodgkin-Huxley model that can predict the frequently observed linear dependence of spiking rates on temperature in warm-sensitive neurons. Additionally, we present data showing how neurons adapt to varying temperatures over time, along with evidence of hysteresis in many temperature-sensitive neurons.

BP 34.4 Fri 12:30 H43

Position-Dependent Non-Markovian Effects Improve Protein

Folding Simulations — •Lucas Tepper, Cihan Ayaz, Benjamin Dalton, and Roland Nezt — Freie Universität Berlin

It's common to project a protein's full atomic resolution onto a one-dimensional reaction coordinate to capture key aspects of its folding process. As a direct consequence of this dimensionality reduction, non-Markovian memory effects emerge. Accounting for memory effects in the framework of the generalized Langevin equation (GLE) with linear friction has proven efficient, accurate and insightful. However, recent advances in deriving GLEs with non-linear, position-dependent friction kernels raise questions about their applicability to protein folding simulations. We derive a novel method to extract position-dependent friction kernels from time series data via conditional Volterra equations. When applied to two protein test systems, the position- and time-dependent friction is strongest for long memory times in the folded states, where atoms are tightly packed. Additionally, we propose a novel and numerically efficient GLE simulation setup, confirming the accuracy of the extracted kernels. Compared to linear friction GLE simulations, our results show that position-dependent non-Markovian effects are critical for accurately reproducing protein folding kinetics when using low-dimensional reaction coordinates.

BP 34.5 Fri 12:45 H43

Multicomponent mixtures exhibit a vast nucleation-and-growth regime — •Yicheng Qiang, Chengjie Luo, and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

Phase coexistence is crucial for understanding how cells regulate biomolecular condensates. Despite of the multicomponent and multiphase nature of such condensates, the direct study of coexisting phases is limited to only few components since the parameter space is high-dimensional. So far, no theory provides a direct and concrete estimation of the phase coexistence behavior of multicomponent mixtures. As a first-level description of multicomponent phase behavior, we derive scaling relations for the number of coexisting phases in typical multicomponent mixtures in equilibrium. The scaling relations reveal that the interactions required to have many coexisting phases only scales very weakly with the number of components, whereas the stability analysis of the homogeneous state suggests a much stronger scaling. This discrepancy implies that large parts of the phase diagram of multicomponent mixture are in the nucleation-and-growth regime, where the homogeneous state is locally stable while multiple coexisting phases are preferred energetically. This suggests that multicomponent mixtures can achieve versatility and controllability in phase behavior with moderate interactions, which might be utilized by cells to create or destroy biomolecular condensates.

BP 35: Closing Talk (joint session BP/CPP/DY)

Time: Friday 13:15–14:00 Location: H2

Invited Talk BP 35.1 Fri 13:15 H2

Active control of forces, movement and shape: from biological to non-living systems — •Ulrich S. Schwarz — Heidelberg University, Heidelberg, Germany

Animal cells are highly dynamic and continuously generate force, for example for division, migration and mechanosensing. Their main force generators are myosin II molecular motors, whose activity is precisely controlled by biochemical circuitry. We first discuss how this system can be hijacked by optogenetics, thus that cellular force generation can be controlled in time and space using light. Next, we use active gel theory combined with van der Waals theory for myosin II molecules to demonstrate that cell contractility is sufficient to explain cell migration and that optogenetics can be used to initiate and revert migration. For two myosin II species, we predict the possibility of oscillations. We then move up in scale and analyze force generation in intestinal organoids, which are epithelia with the topology of a sphere. Combining experimental data, image processing and the bubbly vertex model, we show how apico-basal asymmetries can lead to cell extrusion and budding. We finally discuss how force generation and shape changes can be achieved in non-living systems, in particular for nematic elastomers, in which the direction of contraction is imprinted during polymerization and actuation is achieved by temperature control.