

## BP 14: Poster Session II

Active matter; bacterial biophysics; bioimaging; computational biophysics; membranes, vesicles and life-like systems; protein structure and dynamics; single molecule biophysics; statistical physics of biological systems; systems and networks biophysics; FS integrated structural modelling; FS sequence spaces, populations and evolution

Time: Tuesday 18:00–21:00

Location: P2

BP 14.1 Tue 18:00 P2

**Controlling Cell Motility and Morphology by Microscale Stripe Patterns** — •HENRIK GROH and MATTHIAS WEISS — University of Bayreuth, Experimental Physics I, 95447 Bayreuth, Germany

Cells are highly responsive to the architecture of the substrate on which they adhere. In particular, cell morphology and motility can be influenced by providing microstructured adhesion patterns, e.g. fibronectin-coated lanes of varying width, as this determines how cellular adhesion sites form and organize. To study this in more detail, we generated fibronectin-coated lanes through the Primo technique with widths ranging from  $2.5\text{ }\mu\text{m}$  to  $40\text{ }\mu\text{m}$  on which highly migratory breast cancer cells (MDA-MB-231) adhered. As the lane width was changed, cells exhibited significant changes in their morphology, including alterations in aspect ratio and orientation angle relative to the lanes. In addition, the cells' motility, specifically velocity and migration mode composition, underwent pronounced changes as the lane width decreased. Our findings provide important insights into how cell migration might be guided with simple physico-chemical cues and highlight the potential of micro-patterned substrates as a tool for cancer cell migration analyses, possibly providing a core mechanism that underlies cell migration in development and disease.

BP 14.2 Tue 18:00 P2

**Computational Modelling of Active-Polymer Dynamics in Gliding Filamentous Cyanobacteria** — •KRISHNA IYER VADAKKEPUTHANMADOM SUBRAMANIAN<sup>1</sup>, STEFAN KARPITSCHKA<sup>2</sup>, and STEFAN KLUMPP<sup>1</sup> — <sup>1</sup>Georg-August University, Göttingen, Germany — <sup>2</sup>University of Konstanz, Konstanz, Germany

Filamentous cyanobacteria such as *Oscillatoria lutea*, *Kamptoneema animale* and *Nostoc commune* constitute a natural realization of active polymers: long, flexible filaments that self-propel by gliding motility and whose activity can be tuned with light. Dense colonies display a rich repertoire of collective phenomena—nematic lanes, topological-defects, spirals, clusters etc.—yet the physical mechanisms that connect single-filament properties (bending rigidity, propulsion force, reversal rates) to these emergent states remain largely unexplored. We develop a Brownian-dynamics framework, each filament represented as a chain of active particles with tangential self-propulsion and stochastic direction-reversal events, and explore the collective-state phase diagram in the space of activity, rigidity and length of filaments. Through comparisons with experiments, we seek to understand the mechanisms behind reversal events, both at collective and filament levels.

BP 14.3 Tue 18:00 P2

**Filamentous cyanobacteria in model complex environments** — •JAKOB GÖNNENWEIN, ELIAS ILLING, and STEFAN KARPITSCHKA — Fachbereich Physik, Universität Konstanz

Cyanobacteria are pervasive throughout most ecosystems, ranging from open water bodies to porous media like soil or sandstone. Their accelerated growth in a warming climate constitutes rising ecologic and economic threats. Besides harmful blooms in natural water bodies, their degrading effect on buildings and sculptures has been identified as a threat to cultural heritage sites.

In our work we investigate the motility, individual behaviour and collective mechanics of filamentous cyanobacteria. We use well-controlled quasi-two-dimensional model porous media that mimic properties of natural habitats like soil or sandstone, while allowing direct observation of their dispersal characteristics. Using this system, we derive characteristic persistence scales of orientational order and density fluctuations in relation to the porosity parameters of the model medium.

Characterizing their collective behaviour in porous media allows us to understand and potentially mitigate their adverse effects on porous structural materials.

BP 14.4 Tue 18:00 P2

**Motility Modes and Deformation Dynamics in *Trypanosoma brucei*** — •HANNES WUNDERLICH<sup>1</sup>, MARINUS THEIN<sup>2</sup>, LUCAS

BREHM<sup>2</sup>, GEENA EGLMEIER<sup>2</sup>, KLAUS ERSFELD<sup>2</sup>, and MATTHIAS WEISS<sup>1</sup> — <sup>1</sup>Experimental Physics I, University of Bayreuth, Germany — <sup>2</sup>Laboratory of Molecular Parasitology, University of Bayreuth, Germany

*Trypanosoma brucei* is a unicellular parasitic microswimmer whose flagellum-driven motion and cell-body elasticity are essential for navigating host environments and maintaining immune evasion.

Although run-and-tumble dynamics have been described for both the procyclic and bloodstream forms of *T. brucei*, details of motility changes and cell deformation during locomotion remain poorly understood. To address this gap, we performed a comparative analysis of the motility of bloodstream- and procyclic-form trypanosomes in controlled microfluidic environments. Using high-resolution recordings in bulk and in confining single-emulsion droplets (allowing tracking over extended periods), we extracted and analyzed positional trajectories and cell-shape time series. As a result, we reveal marked differences in swimming efficiency and overall motion patterns between the two trypanosome forms. Our findings indicate that cell-body elasticity and deformation play a crucial role in motility and may be directly relevant for biological processes such as surface-protein exchange.

BP 14.5 Tue 18:00 P2

**A microfluidic device for probing microbial adhesion phenotypes in light and flow gradients** — •FLORIAN BÖHME and OLIVER BÄUMCHEN — University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany

The unicellular photosynthetic microbe *Chlamydomonas reinhardtii* has naturally evolved the ability to unspecifically adhere to surfaces under sufficient illumination with blue light [1]. Their natural habitats are porous, liquid-infused soil and temporary pools. Thus, the cells regularly experience spatiotemporal light variations as well as external flows. *Chlamydomonas* employs its two cilia to firmly attach to surfaces, a mechanism which is hypothesized to sustain a stable photosynthetic yield while providing protection from external flows at low energetic costs.

We mimic such complex natural habitats by creating artificial microscale flow systems with tailored light and fluid flow conditions. Our microfluidic devices entail sections featuring continuous light-intensity gradients of certain wavelengths. At the same time the cells may experience external flows through precise pressure control in the channels. This allows for quantifying population statistics of microbial adhesion phenotypes in terms of threshold intensities of individual light switches and adhesion strengths during exposure to external flows. Our microfluidic devices can be employed for the high-throughput screening of adhesion phenotypes of wild-type and genetically modified photosynthetic microorganisms.

[1] R. Catalan et al., *Soft Matter* **19**, 306 - 314 (2023).

BP 14.6 Tue 18:00 P2

**Active stresses induce bending instabilities and oscillatory dynamics in semiflexible filaments** — •SREEHARI CHOORIKKAT, JONAS BOSCHE, LUDGER SANTEN, and REZA SHAEBANI — Theoretical Physics and Center for Biophysics, Saarland University, 66123 Saarbrücken, Germany

Despite their high structural rigidity, cytoskeletal filaments can undergo large deformations driven by active stresses generated by motor proteins. We investigate this phenomenon by developing a two-dimensional model in which a discretized filament interacts with an underlying array of molecular motors. Using Monte Carlo simulations, we show that stochastic motor binding and unbinding events can produce a wide range of deformation patterns, including bending, buckling, knot formation, and oscillatory motion. We characterize these dynamical regimes by analyzing the time-resolved mean curvature and by determining how the frequency and amplitude of oscillations depend on key physical parameters such as filament length, bending stiffness, and motor density. Our results delineate the parameter space that supports robust, sustained oscillations and clarify how the coupling

between motor activity and filament mechanics generates dynamical instabilities.

BP 14.7 Tue 18:00 P2

**Modeling host-pathogen interactions via stochastic simulations and neural network-driven Bayesian inference** — •SOHAM MUKHOPADHYAY<sup>1</sup>, JONATHAN POLLOCK<sup>2</sup>, DAVID VOEHRINGER<sup>2</sup>, and VASILY ZABURDAEV<sup>1</sup> — <sup>1</sup>MPZPM, Erlangen, Germany — <sup>2</sup>Department of Infection Biology, University Hospital Erlangen, Friedrich-Alexander University Erlangen, 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 of anti-helminth immune responses are often not well-understood. Taking the murine hookworm *N. brasiliensis* as our experimental system, we develop a mechanistic model that describes the parasite load in different host organs — which the parasite migrates through over the course of its lifecycle — as a function of time. We abstract infection progression as a state-transition process and simulate it via kinetic Monte Carlo, thereby linking the infective dose of larvae to the number of eggs shed to the environment by adult worms from the host intestines, which can then be compared to experimental data. To infer model parameters — the various transition rates — from experimental data, we employ emerging techniques from the domain of neural network-driven Bayesian inference to infer the posterior probability distribution of parameters conditioned on data. Using this model and inference framework, we plan to compare the population dynamics for different immune perturbations.

BP 14.8 Tue 18:00 P2

**Structural Analysis of Cyanobacterial Monolayers** — •RODEWALD LARS and KARPITSCHKA STEFAN — Department of Physics, University of Konstanz, Germany

Cyanobacteria are interesting organisms from several perspectives e.g., due to their ecological importance and biotechnical potential but also as model active matter systems as they constitute active polymers that exhibit a wide variety of collective behavior.

Here we investigate dense quasi-2-dimensional layers of filaments and analyze the patterns that emerge from their motility and mutual interactions. In contrast to molecular systems here the complete microstate of the system can be accessed by optical microscopy, which allows for a more complete understanding and description of the global dynamics and structures including nematic and polar order parameters and defect formation.

In this contribution we discuss the design of a confining structure to generate monolayers while providing a healthy environment allowing for long term experiments. Using this structure we investigate the impact of light intensity on the behavior of the individual cyanobacteria and therefore the structures present the associated emerging order in the monolayer.

BP 14.9 Tue 18:00 P2

**Mathematical modeling of larvae motility in complex environments** — •SREYA CHATTERJEE<sup>1</sup>, JHANVI H. PATEL<sup>2</sup>, DAVID VOEHRINGER<sup>2</sup>, and VASILY ZABURDAEV<sup>1</sup> — <sup>1</sup>MPZPM, Erlangen, Germany — <sup>2</sup>Department of Infection Biology, University Hospital Erlangen, Friedrich-Alexander University Erlangen, Germany

*N. brasiliensis* is one of the most widely-studied helminth parasites due to the relatively simple life cycle for parasite production and its ability to be used in animal models, especially rodents. The larvae mature into adult worms in the lumen of the small intestine, which is composed of mucus produced by goblet cells. Studying their interactions with the surrounding host tissue will help us understand how helminths trigger and modulate immune responses. The mucus layer of the extracellular matrix is viscoelastic which influence their motility. We model these adult worms as active agents exhibiting persistent motion within this viscoelastic environment. To capture their dynamics, we formulate the problem using the well-established framework of Active Brownian Particles (ABPs). As a first step, we study the behavior of a simple system of two ABPs connected by a spring through analytical approaches as well as numerical simulations. Next we will extend this model to simulate N-particles connected by springs to capture a more realistic model of the movement of the worm in viscoelastic environment.

BP 14.10 Tue 18:00 P2

**Modeling the aging dynamics of confluent endothelial cells** — •ANSELM HOHLSTAMM, ANDREAS DEUSSEN, STEPHAN SPEIER, and PETER DIETERICH — Institut für Physiologie, TU Dresden

Coordinated movements of endothelial cells are essential for maintaining the barrier function of blood vessels while adapting to disturbances. Understanding the underlying dynamics of these movements can provide valuable insights into the complex biological processes and help to detect changes under pathophysiological conditions. Therefore, we cultured human umbilical vein endothelial cells and stained their nuclei to enable cell tracking. We obtained several tens of thousands of cell paths with durations of up to 48 hours (dt=10 min). Bayesian inference was applied to estimate model parameters and probabilities. Our analysis revealed an age-dependent reduction of mean cell velocities, with cells never coming to a complete standstill. Furthermore, the velocity autocorrelation function indicated correlated movement patterns that persist for approximately 1-2 hours and may be linked to the movements of neighboring cells. The active motion is further influenced by strong repulsive cell-cell interactions, which become particularly relevant shortly after cell division. By combining elements of generalized stochastic processes and cell-cell-interactions, we constructed models that integrate these characteristics and generate collective dynamics in simulations similar to those observed in experiments. In summary, our study provides a comprehensive characterization of endothelial cell movement dynamics and develops a stochastic model that can be used for future simulations and predictions.

BP 14.11 Tue 18:00 P2

**Mechanosensing by active singularities** — •FABIAN KNÜPFER<sup>1</sup>, JONAS NEIPEL<sup>1,2</sup>, and FRANK JÜLICHER<sup>1</sup> — <sup>1</sup>Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — <sup>2</sup>Max Planck Institute for Molecular Cell Biology and Genetics, Dresden, Germany

During the development of an animal, the self-organized formation of chemical patterns establishes the body plan, defining body axes as well as the midline. However, the overall symmetry of an embryo is typically broken before, in particular due to environmental cues. Here we investigate how mechanical cues can control pattern formation. Motivated by the egg-shell that confines various embryos, we consider a rigid heterogenous substrate coupling to an active fluid surface. We focus on localized centers of mechanical activity, i.e. multipoles and topological defects of the active stress field. We ask how variations in friction and substrate curvature impact on the movement of such active singularities. We show that monopoles of isotropic active tension are advected towards maxima in friction. We then discuss how on a curved surface gradients in Gaussian curvature map to friction gradients to explain the localization of stress multipoles in anisotropic geometries. Finally, we explore how in an active nematic, topological defects move along gradients in friction and substrate curvature.

BP 14.12 Tue 18:00 P2

**Swimming With and Against Confined Microscale Flows** — •VISHU SAINI and MARISOL RIPOLL — Theoretical Physics of Living Matter (IAS-2), Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

Bacteria in real-world settings are typically navigating heterogeneous porous media, such as soil [1]. Such environments involve a complex interplay between geometric confinement and fluid flow [2], which can be understood as networks of channels with varying cross sections [3]. By means of Brownian Dynamics simulations, we investigate the properties of microswimmers in the presence of both confinement and flow to identify universal mechanisms that microorganisms employ to traverse complex environments. Since self-propelled particles tend to accumulate at the walls, the strength of the flow will determine the upstream or downstream nature of swimming. This will be importantly modified by the intrinsic rotational noise of the self-propelled and the channel width, which is known to vary together with the geometric characteristics of the media. The interaction between self-propelled particles will also importantly affect the dynamics with the formation of percolating clusters. We systematically characterize these dynamics for varying flow strengths and channel sizes, as often encountered in soil-like porous environments.

[1] Bhattacharjee et al (2019). *Nature communications*, 10(1), 2075.  
 [2] Conrad, J. C et al. *Annual review of chemical and biomolecular engineering*, 9(1), 175-200. [3] Monteiro et al. *Commun Biol* 8, 662 (2025).

BP 14.13 Tue 18:00 P2

**Synthesis and characterization of platinum (pt)-decorated se-tio2@fcnts nanocomposite and their photocatalytic antibacterial mechanism** — •ASIF KAMAL<sup>1</sup>, AKHTAR MUNIR<sup>2</sup>, JINGUANG YANG<sup>3</sup>, and YINGWEN WANG<sup>4</sup> — <sup>1</sup>Department of Plant Sci-

ences Quaid-i-Azam University Islamabad, 45320 Islamabad, Pakistan. — <sup>2</sup>Department of Chemistry, Quaid-i-Azam University Islamabad, 45320 Islamabad, Pakistan. — <sup>3</sup>Key Laboratory of Tobacco Pest Monitoring, Controlling and Integrated Management, Tobacco Research Institute of Chinese Academy of Agricultural Sciences, Qingdao 266101, China: — <sup>4</sup>Key Laboratory of Tobacco Pest Monitoring, Controlling and Integrated Management, Tobacco Research Institute of Chinese Academy of Agricultural Sciences, Qingdao 266101, China:

The development of efficient and sustainable antibacterial agents is crucial to address the growing threat of multidrug-resistant pathogens. In this study, we report the synthesis and characterization of a novel nanocomposite Pt-decorated selenium-doped titanium dioxide supported on functionalized carbon nanotubes (Pt/Se-TiO<sub>2</sub>@FCNTs) with enhanced photocatalytic antibacterial performance under visible light. This new material was synthesized through sol gel method by in situ pt NPs decoration to achieve uniform dispersion and strong interfacial coupling between the components. Comprehensive characterization using XRD, TEM, SEM-EDS, FTIR, Raman, XPS and UV confirmed successful Se doping, Pt decoration, and improved optical absorption in the visible range. The photocatalytic antibacterial activity was evaluated against *E. coli* and *Ralstonia solanacearum*.

BP 14.14 Tue 18:00 P2

**Laser-cell interactions in a microorganism model: Influence of irradiation with 1064 nm on *E. coli*** — •KATJA SCHMITZ and BEATRIX KONERMANN — Trier University of Applied Sciences, Trier, Germany

Lasers are being used more and more in sensor technology, including in biotechnological applications such as fermentation monitoring. However, the biological impact of laser radiation on microorganisms is not fully understood. Depending on the wavelength, the radiation can induce DNA damage, protein denaturation, or thermal effects, which can inhibit growth or kill cells. Additional parameters, such as irradiation duration and intensity, also influence these interactions.

This study investigates the effects of a 1064 nm laser on the growth and metabolism of *E. coli* under different irradiation conditions. An *E. coli* culture was exposed to a 100 mW laser radiation with variable irradiation times. After treatment, the samples were either cultivated immediately or returned to the culture medium. Growth behavior was evaluated by determining total and viable cell counts, which were then compared to those of untreated reference samples.

Initial results showed no detectable influence of 1064 nm irradiation on cell growth or metabolic processes. A literature review was conducted to contextualize these findings and summarize the reported positive, negative, and neutral effects of laser exposure on microorganisms. These results contribute to a more detailed understanding of laser-cell interactions and highlight the need for further research, particularly regarding wavelength- and organism-specific effects.

BP 14.15 Tue 18:00 P2

**Agent-based modeling of short range cell-cell communication** — •RICARDO SANTANDER<sup>1,3</sup>, NOAM GOLAN<sup>2</sup>, LIOR KREINDLER<sup>2</sup>, AVIGDOR ELDAR<sup>2</sup>, and VASILY ZABURDAEV<sup>1,3</sup> — <sup>1</sup>Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — <sup>2</sup>School of Molecular Cell Biology & Biotechnology Tel Aviv University, Israel — <sup>3</sup>Friedrich-Alexander-Universität, Erlangen, Germany

We use agent-based simulations to model synthetic gene regulatory networks that mediate short-range cell-cell communication in bacterial monolayers. These circuits couple intracellular dynamics of transcription factors and inhibitors with extracellular concentration fields driven by diffusion, secretion, and uptake of signaling peptides. Individual bacteria are represented as elongating, dividing capsules that act as point-like sources and sinks shaping the extracellular concentration field. The model is nondimensionalized to expose key parameter groups that govern the balance between secretion, import, diffusion, and dilution. Simulations reproduce the influence of nearby inhibitor-producing cells on their neighbors observed in microfluidic experiments and provide detailed insight into how spatial organization and transporter-driven accumulation control signaling range, spatial patterns, and circuit behavior in dense bacterial populations

BP 14.16 Tue 18:00 P2

**Effects of extracellular DNA on material properties of bacterial biofilms** — •MANDUS ALDAG, ISABELLE WIELERT, STEPHAN WIMMI, and BERENIKE MAIER — Institute for Biological Physics, University of Cologne

Many bacterial species form spatially structured biofilms that protect the bacteria from external stresses. In *Neisseria gonorrhoeae*, a human pathogen, early biofilms are characterized by the formation of spherical colonies with liquid-like local order via active attractions between single cells. An important component of biofilms is extracellular DNA (eDNA), that is predominantly released from lysed cells and is proposed to have biofilm-stabilizing properties. Here, we use a combination of confocal microscopy, laser tweezers and tolerance assays to explore the spatial distribution of eDNA and how it affects structure, dynamics and attractive forces in gonococcal colonies. We find that after 16h of growth, *N. gonorrhoeae* colonies show filamentous, network-like eDNA structures, that can span over large parts of the colony and often interconnect lysed cells. Treatment with DNase prevents the formation of the eDNA network while the spherical colony shape is maintained. Furthermore, we find that the presence of eDNA is associated with a lower bacterial within-colony motility, compared to DNase-treated colonies. The results suggest that even though gonococcal colonies can still form in DNase presence, eDNA affects the cohesive properties of cells within biofilms which potentially influences the biofilm's susceptibility to antibiotics.

BP 14.17 Tue 18:00 P2

**Probing Bacterial Adhesion on Functionalized Silicon Surfaces Using AFM-Based Single-Cell Force Spectroscopy** — •HANNAH HEINTZ, HENDRIK HÄHL, and KARIN JACOBS — Experimental Physics & Center for Biophysics, Campus E2 9, 66123 Saarbrücken, Germany

Understanding bacterial adhesion to solid surfaces is crucial for biomedical as well as technical applications ranging from implants to antifouling strategies. In this study, we investigate how chemical functionalization and nanoscale roughness influence microbial attachment. We employed silicon surfaces that were modified by (i) coating with octadecyltrichlorosilane (OTS) to render them hydrophobic, (ii) preconditioning with a protein film of the hydrophobin HFBI from *Trichoderma reesei*, and (iii) controlled etching with hydrofluoric acid to introduce varying roughness levels. Adhesion forces of *Staphylococcus aureus* and *Shewanella oneidensis* were quantified using Atomic Force Microscopy (AFM)-based Single-Cell Force Spectroscopy (SCFS), employing both polydopamine-mediated and FluidFM vacuum-based cell immobilization. Complementary AFM and confocal microscopy enabled simultaneous characterization of topography, elasticity, and cell wall architecture. Our results reveal distinct adhesion profiles depending on surface chemistry and bacterial species, highlighting the interplay between hydrophobicity and roughness. These findings provide mechanistic insights into biointerface design and pave the way for tailored surface engineering to control microbial colonization.

BP 14.18 Tue 18:00 P2

**Exploring Chemotaxis in Magnetotactic Bacteria: A Biophysical Approach** — •DIEGO ROESCH — Institut de Biosciences et Biotechnologies d'Aix-Marseille, Aix en Provence, France

Magnetotactic bacteria (MTB) navigate complex microenvironments by integrating magnetic, chemical, and physical cues. Although magnetotaxis and aerotaxis have been extensively studied, the mechanisms governing chemotaxis in MTB remain largely unexplored, particularly at the level of the bacterial flagellar motor. This work aims to establish a quantitative steady-state model of motor dynamics in Magnetospirillum gryphiswaldense (MSR-1) as a foundation for studying how the motor adapts to and integrates chemical stimuli.

Using tethered-cell assays, high-speed recording, and a custom Python analysis pipeline, individual MSR-1 motors were characterized, revealing three well-defined rotational states: counterclockwise (CCW), clockwise (CW), and pausing. MSR-1 motors exhibited frequent directional reversals and extensive time spent in transient failed-switch pauses, whereas genuine long pauses formed rare but highly persistent states following lognormal distributions, likely reflecting regulatory or mechanistic resets of the motor.

Switching intervals, long pauses, and most run durations follow non-Poissonian, lognormal-like statistics, suggesting structured rather than memoryless regulation. Since MSR-1 possesses two polar flagella, this framework also opens the way to investigate the synchronicity and coordinated behavior of both motors under chemical stimulation.

BP 14.19 Tue 18:00 P2

**Controlling transport for RNA enrichment in alkaline hydrothermal vents at the emergence of life** — •MONA B. MICHELSEN<sup>1</sup>, ALMUTH SCHMID<sup>2</sup>, DIETER BRAUN<sup>2</sup>, and KAREN ALIM<sup>1</sup>

—<sup>1</sup>Theory of Biological Networks, School of Natural Sciences, Technical University of Munich, Garching, Germany —<sup>2</sup>Systems Biophysics, Ludwig Maximilians University, Munich, Germany

Reactive mineral surfaces within alkaline hydrothermal vents (AHVs) at the prebiotic ocean floor are compelling candidates for mediating the accumulation and stabilization of early biomolecules such as RNA. The intricate hierarchical architecture of AHVs, featuring central conduits branching into finely ramified networks, creates dynamic microenvironments that may promote selective adsorption of RNA onto mineral surfaces and enhance local concentrations through flow-driven accumulation. These mineral-RNA interactions could have influenced both the persistence and the catalytic potential of primitive RNA species, potentially facilitating steps toward replication and evolution.

In this project, we apply microfluidics to construct quasi-2D analogues of hydrothermal vents in the laboratory, enabling direct observation of mineral precipitation, flow patterns, and RNA transport under controlled chemical and physical conditions. This approach allows us to investigate how mineral surfaces and flow dynamics influence RNA accumulation and the potential for mineral-assisted RNA catalysis and replication in prebiotic environments.

BP 14.20 Tue 18:00 P2

**Molecular Dynamics Simulations as a tool to investigate the impact of novel imidazole-based cholesterol analogs in lipid bilayers** — •CLARA RICKHOFF and ANDREAS HEUER — Institut für Physikalische Chemie, Universität Münster, Münster, Germany

In biological membrane systems of eukaryotic cells, the cholesterol plays an important role, impacting for example the fluidity and structure of the membrane. To gain a deeper understanding of the behaviour of cholesterol a range of analogs were developed to add functionalities required for lab experiments such as fluorescence to the sterol. In order to investigate cholesterol via these tools, it is essential that the analogs show a similar behaviour to that of the wildtype molecule. In a previous study a similar behaviour was observed between a non-charged imidazole-based cholesterol analog (CHIM-N) and cholesterol itself [1].

The present study focuses on a novel group of imidazole-based cholesterol analogs with a more flexible linker between imidazolium and cholesterol and a fully retained cholesterol backbone. Via Molecular Dynamics (MD) Simulations it can be assessed how accurate these new analogs mimic cholesterol in terms of order parameter, tilt angle and position within the membrane. Furthermore, a comparison of the different new analogs as well as with the molecules already applied in cells can be made.

[1] M. Pierau et al, Langmuir 2025, 41 (17), 10991-11002

BP 14.21 Tue 18:00 P2

**Modelling genome condensation and membrane bending in SARS-CoV-2** — •NILS O. WINKLER, SARAH M. SEIBERT, FALKO ZIEBERT, and ULRICH S. SCHWARZ — Institut Theoretische Physik & BioQuant, Uni Heidelberg

While many enveloped RNA-viruses use a rigid protein capsid to package and protect their genome, SARS-CoV-2 uses a high density of the transmembrane protein M to structurally reinforce its membrane, which then bends around the viral genome condensed by the cytosolic protein N. Interestingly, the RNA-genome seems to be further subdivided into smaller subunits, leading to a nested egg structure. We theoretically study the energetics of this situation by minimizing appropriate energy functions for genome condensation, membrane bending, droplet wetting and wrapping. In particular, we investigate which of these energy contributions can explain the nested egg structure as observed experimentally.

BP 14.22 Tue 18:00 P2

**Modelling Wave Propagation on Monolayers** — •PHILIPP ZOLTHOFF and JAN KIERFELD — TU Dortmund University, Dortmund, Germany

Recent experimental advances have enabled precise studies of pressure wave propagation through monolayers at the air-water interface, triggered by light-induced conformation changes of embedded azobenzenes. We model wave generation and propagation using a fractional Lucassen-type wave equation and compare experimental results on pulse shape and pulse propagation in detail with numerical simulations in order to describe experiments quantitatively and unravel the influence of possible non-linearities and different rheological monolayer models. Particular attention is paid to the question how the influence

of non-linearities and rheology changes for different states of the monolayer, i.e., in different regions along its Langmuir isotherm.

BP 14.23 Tue 18:00 P2

**A synthetic flow system for modelling the vascular margination effect using microbeads** — •TERESA M. MAUNZ, ALEXANDRA BIENAU, FRIEDRICH SIMMEL, and KAREN ALIM — School of Natural Sciences, Technical University of Munich, Germany

The margination effect in the blood vasculature causes particles to migrate toward the blood vessel walls due to interactions with red blood cells (RBCs). Margination plays an important role in particle-based drug delivery targeted at the vascular endothelium, which requires contact with the endothelium for delivery. While margination has been studied with simulations and (some) experiments, how to control margination for synthetic particles is underexplored and requires thorough experimental testing of multiple variable parameters. Here, we present a synthetic microfluidic system dedicated to investigating the margination effect. The base system consists of a microfluidic channel carrying a binary suspension of beads, mimicking RBCs and marginating particles. Physiological conditions are emulated by tuning parameters that have been predicted to be crucial for the emergence and prominence of the margination effect, such as vessel diameter, RBC volume fraction, RBC deformability, the size ratio between RBCs and particles, and flow characteristics. We anticipate that our system will contribute to identifying key parameters that enable the margination effect, thereby improving our understanding of blood flow and facilitating the development of future drug delivery testing models.

BP 14.24 Tue 18:00 P2

**Effects of perfluorocarbons on lipid monolayers and protein adsorption** — •JAQUELINE SAVELKOULS<sup>1</sup>, MICHAEL PAULUS<sup>1</sup>, CHRISTIAN THIERING<sup>1</sup>, MICHELLE DARGASZ<sup>2</sup>, LENA FRIEDRICH<sup>1</sup>, MIKE GEORGE<sup>1</sup>, PRASHANT HITAISHI<sup>3</sup>, SVENJA HÖVELMANN<sup>3,4</sup>, OLEG KONOVALOV<sup>5</sup>, ERIC SCHNEIDER<sup>1</sup>, GORDON SCHOLZ<sup>1</sup>, CHEN SHEN<sup>4</sup>, and METIN TOLAN<sup>1</sup> — <sup>1</sup>Technische Universität Dortmund, Germany — <sup>2</sup>Universität Siegen, Germany — <sup>3</sup>Christian-Albrechts-Universität zu Kiel, Germany — <sup>4</sup>DESY, Hamburg, Germany — <sup>5</sup>ESRF, Grenoble, France

Lipid monolayers serve as biomimetic models to study structural and functional aspects of protein-membrane interactions, which are essential for understanding physiological functions. Investigating how perfluorocarbon (PFC) effects on these interactions may aid new therapeutic strategies. This study examines the influence of various PFCs on structural changes of lung-surfactant-like DPPA and DPPC monolayers at different initial surface pressures, as well as on the adsorption behavior of surface-active proteins. Experiments were conducted at beamlines ID10 (ESRF, Grenoble) and P08 (PETRA III, Hamburg) under ambient conditions using a combined grazing incidence X-ray diffraction and X-ray reflectivity study. The results demonstrate that the effect of the PFCs on the lipid structure and protein adsorption depends on the chemical characteristics of the PFCs, the lipid type, and the lipid phase. This work will discuss how the adsorption of PFCs at the membrane promotes protein association.

BP 14.25 Tue 18:00 P2

**Local dynamical properties of lipid bilayers using Scanning Ion Conductance Microscopy (SICM)** — •ERIC LIEBERWIRTH<sup>1</sup>, FRANZISKA DORN<sup>1</sup>, REGINA LANGE<sup>1</sup>, UNA JANKE<sup>2</sup>, MIHAELA DELCEA<sup>2</sup>, INGO BARKE<sup>1</sup>, and SYLVIA SPELLER<sup>1</sup> — <sup>1</sup>Physics of Surfaces and Interfaces, Institute of Physics & LLM, University of Rostock, Germany — <sup>2</sup>Biophysical Chemistry, Institute of Biochemistry, University of Greifswald, Germany

To determine dynamical properties of lipid bilayers, various experimental methods have been established, e. g. contour analysis and fluctuation spectroscopy. Based on HELFRICH theory from 1973 [1], bending rigidity and membrane tension of lipid bilayers can be derived. We demonstrate a local measurement approach by Scanning Ion Conductance Microscopy (SICM) on Giant Unilamellar Vesicles (GUVs) for evaluation of dynamic lipid bilayer properties. Using a nanopipette controlled via a feedback loop to maintain constant membrane-tip distance, we record time traces of local membrane height fluctuations with nanometer precision. In a contour analysis like approach [2], we obtain a bending rigidity of a few  $k_B T$  and membrane tension of a few  $\mu\text{Nm}^{-1}$ . Computation of the power spectral density (PSD) based on [3] combined with a global-local fit provides a second evaluation route with same data set, yielding in similar results. Differences and limitations of both methods are discussed.

[1] W. Helfrich, *Zeits. für Naturfor.* 28c (1973), p. 693-703  
 [2] J. F. Faucon et al., *J. Phys. France* 50 (1989), p. 2389-2414  
 [3] T. Betz & C. Sykes, *Soft Matter* 8 (2012), p. 5317-5326

BP 14.26 Tue 18:00 P2

**Influence of PLIN5 and Lipid Composition on Lipid Droplet Contact Sites with other Organelles** — •MAHSA MOHAMMADIAN, SHIMA ASFIA, and RALF SEEMANN — Department of Experimental Physics and Center for Biophysics, Saarland University, Saarbrücken, Germany

Lipid droplets (LDs) maintain cellular lipid homeostasis through dynamic interactions with other organelles. Understanding how these contact sites form is crucial for uncovering the mechanisms of lipid exchange and signaling. In this study, we used an *in vitro* model to investigate how lipid composition and the LD-associated protein perilipin 5 (PLIN5) influence contact formation between an LD monolayer and a bilayer membrane. Artificial LDs consisting of triolein and coated with either a DOPE or DOPC monolayer containing PLIN5 or not were incubated with large unilamellar vesicles (LUVs) that mimic the bilayer membrane of the organelle. Using double fluorescence labeling of the LUV bilayer and the core, we can distinguish between fusion of the LUV bilayer with the LDs and stable attachment of LUVs to the LD's surface. Our results show that the probability of fusion between LDs and LUVs is greatly increased for DOPE-coated LDs, while PLIN5 promotes the stable attachment of LUVs to the LD's surface and prevents fusion. These observations illustrate how certain lipid and protein components can modulate contact formation between LDs and membranes in a controlled *in vitro* system, and provide a basis for future studies on the molecular mechanisms of organelle communication.

BP 14.27 Tue 18:00 P2

**Elucidating the dynamics of DNA-based Transmembrane Receptors through Molecular Dynamics Simulations** — •CYRILLE NGUELDJOU TAHABO<sup>1</sup>, DORUK BAYKAL<sup>2</sup>, LORENA BARANDA PELLEJERO<sup>2</sup>, ANDREAS WALTHER<sup>2</sup>, and LUKAS STELZL<sup>3,4</sup> — <sup>1</sup>Institute of Physics, University of Johannes Gutenberg, Mainz, Germany — <sup>2</sup>Department of Chemistry, University of Johannes Gutenberg, Mainz, Germany — <sup>3</sup>Institute of Molecular Physiology, University of Johannes Gutenberg, Mainz, Germany — <sup>4</sup>Institut of Molecular Biology, Mainz (IMB), Germany

Building an artificial cell is an essential step to creating artificial life-like systems and a critical step in this endeavour is to design molecular systems which enable the communication of an artificial cell with its environment. Such artificial life-like systems hold great promise for biomedical engineering. By mimicking biological mechanisms to enable the transmission of information from the exterior of artificial cells across membranes to their interior, we will contribute to creating new artificial life-like systems and gain insights to essential biological information processing mechanisms and advance simulation method development, using an atomistic molecular dynamics and Coarse Grained simulations approaches, who can be synthesized to function as receptors in artificial life-like systems. we study DNA attached to an anchor insert in lipid membranes. In the simulations we investigate how Anchor interacts with the membranes and how DNA-Anchor changes local membrane structure.

BP 14.28 Tue 18:00 P2

**Ray-based simulation and experimental analysis of red blood cell imaging in brightfield microscopy**

— •AARON KREIS, SARAH TABEA HERMES, THOMAS JOHN, and CHRISTIAN WAGNER — Experimental Physics, Saarland University

The interpretation of brightfield microscopy images of red blood cells (RBCs) requires a quantitative understanding of how light propagates through their biconcave geometry. We present a numerical ray-tracing framework that models refraction and reflection at the cell–medium interface according to Snell's and Fresnel's laws, explicitly reproducing the optical configuration of a brightfield microscope. The simulated intensity distributions show excellent quantitative agreement with experimentally measured axial intensity profiles acquired using a conventional inverted microscope. This confirms that geometrical optics adequately describe light propagation through RBCs, as diffraction effects remain negligible for micrometer-scale objects. The approach enables label-free prediction of contrast and focus-dependent image formation, paving the way for future quantitative assays of single-cell oxygenation and advanced label-free imaging.

BP 14.29 Tue 18:00 P2

**Photothermal imaging of autofluorescent retinal pigment epithelium (RPE) granules** — •SICHENG TIAN<sup>1,2</sup>, MARYAM ALI<sup>1,2</sup>, HANAN ALDERZY<sup>1,3</sup>, CHRISTOPH KRAFFT<sup>1,2</sup>, MARTIN HAMMER<sup>1,3</sup>, and DANIELA TÄUBER<sup>1,2</sup> — <sup>1</sup>Friedrich Schiller University Jena — <sup>2</sup>Leibniz Institute of Photonic Technology, Jena — <sup>3</sup>Jena University Hospital, Jena, Germany

The retinal pigment epithelium (RPE) plays an important role in the photocycle. RPE cells contain varied amounts of micrometer-sized autofluorescent granules, including melanosomes (M), lipofuscin (L) and melanolipofuscin (ML), whose distribution varies throughout the RPE layer and with increasing age. Non-invasive fundus autofluorescence is used for clinically monitoring the distribution of L and ML. Specific alterations in the distribution of L, ML and M are linked to age-related macular degeneration (AMD)[Bermond et al., IOVS, 2020, 61, 35]. In spite of their importance, their chemical composition is not fully understood. Mid-IR Photo-induced Force Microscopy (PiF-IR) can provide a chemical evaluation of cell and organelle surfaces with less than 5 nm spatial resolution [Ali et al., *Anal. Chem.*, 2025, 97, 23914] by combining powerful infrared illumination with mechanical detection using atomic force microscopy (AFM-IR). We utilized PiF-IR for the investigation of isolated M in a dried droplet. We complemented our study by sub-micron photothermal images using Optical Photothermal Infrared spectroscopy (O-PTIR) under illumination at visible wavelengths. We compare the results to PiF-IR spectra and conventional Fourier-transform IR spectra obtained on membrane phospholipids.

BP 14.30 Tue 18:00 P2

**Multimodal imaging with light microscopes and scanning small angle X-ray scattering** — •BORAM YU<sup>1</sup>, MANGALIKA SINHA<sup>1</sup>, RITA MENDES DA SILVA<sup>1,2</sup>, ULRIKE RÖLLEKE<sup>1</sup>, MANFRED BURGHAMMER<sup>2</sup>, and SARAH KÖSTER<sup>1</sup> — <sup>1</sup>Institute for X-Ray Physics, University of Göttingen, Germany — <sup>2</sup>The European Synchrotron, Grenoble, France

Imaging biological cells using X-rays is a complementary approach to electron and fluorescence microscopy due to their high penetration depth and the possibility for label-free imaging. One such technique is scanning small angle X-ray scattering (SAXS), which enables the acquisition of a real-space overview image with moderate resolution and reciprocal-space information with high resolution of cells in aqueous environment. However, intracellular structures in aqueous environment are very sensitive to radiation; therefore, the investigation of such damage requires additional imaging techniques beyond scanning SAXS. We present a scanning SAXS configuration, which integrates a mobile fluorescence microscope and an on-axis bright field microscope with a microfluidic sample chamber. The microfluidic sample chamber is compatible with X-ray measurement, as well as two microscopes, owing to its very thin design. While the fluorescence microscope enables obtaining correlative images before and after X-ray scanning within a short time span, the bright field microscope produces bright field images simultaneously during the scan. Our approach provides complementary information on specimens to X-ray measurements, thereby demonstrating its applicability in various fields.

BP 14.31 Tue 18:00 P2

**Receptor-Mediated Binding Kinetics of Ligand-Functionalized Lipid Nanoparticles for Targeted mRNA Delivery** — •TIANYI CAO — Faculty of Physics and Center for NanoScience, Ludwig Maximilians University, Munich 80539, Germany

For targeted mRNA delivery, lipid nanoparticles (LNPs) are functionalized with PEG-lipid tethers that display affinity ligands—such as full antibodies, Fab fragments, or peptides—to enable receptor-specific cell binding.

We establish a quantitative single-cell binding assay to characterize these receptor-mediated interactions using functionalized LNPs. Using time-lapse live-cell imaging on single-cell arrays (LISCA), we track individual particles via fluorophore-labeled lipid components incorporated directly into the LNP membrane. We systematically vary the molar fraction of functionalized PEG-lipids to quantify how ligand density influences binding probability and saturation behavior.

From these trajectories we extract apparent on-rates, binding capacities, and cell-to-cell variability arising from heterogeneous receptor expression. Under controlled shear flow, we distinguish diffusion-limited from reaction-limited binding and quantify how hydrodynamic forces modulate bond formation and stability.

We further extend the framework to multivalent LNPs carrying mixtures of different ligands that target distinct receptors on the same cell. This assay provides a mechanistic, single-cell-resolved readout of receptor-mediated LNP binding, enabling rational optimization of selective mRNA delivery formulations.

BP 14.32 Tue 18:00 P2

**Optical properties of red blood cells and refractive index of hemoglobin** — •SARAH TABEA HERMES, AGATHA BELÉN PINTO PINO, THOMAS JOHN, and CHRISTIAN WAGNER — Experimental Physics, Saarland University

As the determination of the oxygen saturation of whole blood is common practice in medicine, the research of the oxygenation state of individual red blood cells (RBCs) remains challenging. When observing RBCs under a light microscope, the image is a composition of absorption as well as refraction (since the refractive index inside the RBC is higher than in the medium) and further depends on the focal plane, see Poster Aaron Kreis. This is important both for determining the composition of the cell via absorption as well as for edge detection because the refraction leads to "ghost edges". It is thus relevant to research the optical properties of RBCs and in particular the refractive index of the hemoglobin inside the RBCs. This allows for better comparison with numerical simulations and enables to precisely match the refractive index of the medium and the RBCs. We will present a detailed measurements about the refractive index of hemoglobin solutions in comparison with literature values.

BP 14.33 Tue 18:00 P2

**Time resolved fluorescence anisotropy of single phalloidin-dye complexed F-Actin fibrils: MD simulation and experiments** — PHILLIP SEEBER<sup>1</sup>, •SHANGJUN CHENG<sup>1,2</sup>, LUKAS SPANTZEL<sup>1,3</sup>, RAINER HEINTZMANN<sup>1,2</sup>, and DANIELA TÄUBER<sup>1,2</sup> — <sup>1</sup>Friedrich Schiller University Jena — <sup>2</sup>Leibniz Institute of Photonic Technology, Jena — <sup>3</sup>Jena University Hospital, Jena

Phalloidin conjugates are widely used to visualize actin filaments (F-Actin) due to their high binding affinity [1]. Fluorescence polarization imaging adds information on cellular structures known from other approaches [2, 3]. Moreover, super-resolution techniques such as STED and SIM often employ polarization optics. For aligned samples, such as actin filaments, insights in fluorophore orientation and wobbling dynamics will improve the interpretation of experimental results. Here, we apply quantum chemical methods including DFT, TD-DFT and ADC(2) to study the trajectory of the dye's transition dipole moments during thermal fluctuations. We correlate the MD simulations with fluorescence anisotropy measurements acquired using time-resolved fluorescence lifetime imaging (FLIM) and 2D polarization fluorescence imaging (2D-POLIM) [3]. [1] Melak M., Plessner M., et al. Journal of cell science, 2017, 130, 525. [2] Rimoli, C. V., Valades-Cruz C.A., et al. Nat Commun 2022, 13, 301. [3] Camacho R., Täuber D., et al. Communications Biology, 2018, 1, 157.

BP 14.34 Tue 18:00 P2

**Nanomechanical ultrastructure of native skin** — •MARIO ZERSON<sup>1</sup>, MARTIN DEHNERT<sup>1</sup>, PAUL ZECH<sup>1</sup>, MELANIE KNAAK<sup>2</sup>, KORINNA JÖHRENS<sup>2</sup>, MARTIN KAATZ<sup>3</sup>, and ROBERT MAGERLE<sup>1</sup> — <sup>1</sup>Fakultät für Naturwissenschaften, TU Chemnitz — <sup>2</sup>Institut für Pathologie, Klinikum Chemnitz gGmbH — <sup>3</sup>Hautklinik, DRK Krankenhaus Chemnitz-Rabenstein

Native skin has a complex, layered structure across the epidermis and dermis. In this study, we explore the use of atomic force microscopy (AFM) to examine the nanomechanical morphology of skin under controlled relative humidity conditions that maintain water content close to physiological levels. We examined cryosections of native, unfixed rabbit skin with tapping mode AFM and AFM-based nanoindentation measurements. This enables imaging the nanomechanical ultrastructure of the stratum basale in the epidermis and of collagen fibrils in the dermis with 20 nm spatial resolution. The results are compared with optical micrographs of adjacent stained sections of the same specimen and with scanning electron micrographs reported in the literature.

BP 14.35 Tue 18:00 P2

**Red Blood Cell shape classification using curvature flow and spherical harmonics** — •NIKOLAS LERCH, FELIX MAURER, DIANA ÖRÜM, and THOMAS JOHN — Universität des Saarlandes

The morphological characterization of erythrocytes deformed due to pathology or disease has traditionally relied on manual assessment,

which introduces subjective sources of error and hampers the differentiation of closely related morphologies such as echinocytes and acanthocytes. We present an automated method for the objective classification of deformed erythrocytes. The approach employs a bijective mapping of surface curvature onto a reference sphere via curvature flow and decomposes the resulting features into spherical harmonics. The resulting spectral signatures enable the assignment of cells to morphologically distinct clusters. The method is quantitative and reproducible, explicitly identifies transient shapes and transition regions between morphologies, recognizing them as such and distinguishing them from clearly defined class expressions, and thereby opens new perspectives for computer-assisted hematology.

BP 14.36 Tue 18:00 P2

**Diffusion and deoxygenation/oxygenation of hemoglobin solutions in microfluidics** — •AGATHA BELÉN PINTO-PINO, SARAH TABEA HERMES, THOMAS JOHN, and CHRISTIAN WAGNER — Experimental Physics, Saarland University

The observation of red blood cells (RBCs) under bright field microscopy allows the study of how absorption and refraction combine to form image contrast. In this work, we use the absorption of light to investigate the diffusion of hemoglobin in water in microfluidic channels. By analyzing how intensity profiles evolve over time, we characterize the diffusion behavior of hemoglobin in water. The setup will also be used to study the transition from deoxygenated to oxygenated hemoglobin, because the absorptions differ strongly for those states, in particular for different wave length of the light. This study helps for a better understanding of the mechanisms that govern oxygen transport in blood.

BP 14.37 Tue 18:00 P2

**Implementation of NIR excitation and detection in 2D-POLIM setup** — SHANGJUN CHENG<sup>1,2</sup>, •ZILONG HUANG<sup>1</sup>, RAINER HEINTZMANN<sup>1,2</sup>, and DANIELA TÄUBER<sup>1,2</sup> — <sup>1</sup>Friedrich Schiller University Jena — <sup>2</sup>Leibniz Institute of Photonic Technology, Jena

Two-dimensional polarization fluorescence imaging (2D-POLIM) has been used to probe the orientation/rotation of molecules and the Förster resonance energy transfer between closely located chromophores [Camacho et al., Adv. Mat. 2019, 31, 1805671; Camacho et al., Commun. Biol. 2018, 1, 157]. 2D-POLIM can provide full in-plane information on the polarization state of the sample through synchronized control of the excitation and detection polarizations. Near-infrared (NIR) excitation reduces the background from intrinsic auto-fluorescence in cells and tissue samples. Here, we show a stable, precisely controllable excitation polarization of a 785 nm laser. We also demonstrate the potential of 2D-POLIM in imaging and analysis of molecular orientation in the NIR range.

BP 14.38 Tue 18:00 P2

**Metasurfaces for Oblique Plane Microscopy** — •MAIKE KREUTZ<sup>1,2</sup>, MARTIJN MOORLAG<sup>1</sup>, IBNUN NUR AKASH<sup>3</sup>, STEPHAN DAETWYLER<sup>4</sup>, SARA LELEK-GRESKOVIC<sup>5</sup>, IBNUN NUR AKASH<sup>3</sup>, YIJUN WANG<sup>3</sup>, CHIH-YAO HSU<sup>6</sup>, YU-CHUAN CHANG<sup>6</sup>, YAO-WEI HUANG<sup>6</sup>, RETO FOLKA<sup>4</sup>, FLORIAN ENGERT<sup>1</sup>, MARYNA L. MERETSKA<sup>3</sup>, and FABIAN F. VOIGT<sup>1</sup> — <sup>1</sup>MCB, Harvard University — <sup>2</sup>RWTH Aachen University — <sup>3</sup>INT, Karlsruhe Institute of Technology (KIT) — <sup>4</sup>UT Southwestern Medical Center — <sup>5</sup>SCRB, Harvard University — <sup>6</sup>Department of Photonics, National Yang Ming Chiao Tung University

A promising emerging bioimaging technique is oblique plane light-sheet microscopy (OPM), which allows volumetric imaging using a single scan mirror but suffers from significant losses due to its complex optical path. To enhance the light-collection efficiency of OPMs, we propose to integrate optical metasurfaces into the optical path of an OPM. Metasurfaces utilize sub-wavelength nanostructures for manipulation of electromagnetic fields and can be produced with CMOS-compatible technology. By implementing tailored metagrating designs, we aim to reduce losses in single-objective light-sheet setups.

BP 14.39 Tue 18:00 P2

**Lens-free lab-on-chip fluorescence microscopy using angle-stable polariton filters** — •ANJA LINDENAU<sup>1</sup>, ANDREAS MISCHOK<sup>1</sup>, and MALTE GATHER<sup>1,2</sup> — <sup>1</sup>Humboldt Centre for Nano- and Biophotonics, Department of Chemistry, University of Cologne, Germany — <sup>2</sup>School of Physics and Astronomy, University of St Andrews, Scotland

Fluorescence microscopy is an essential tool in biomedical research

but typically relies on complex optical setups with high-numerical-aperture objectives and specialised colour filters, which results in a large footprint and high acquisition costs. Here, we present a modified commercial CMOS image sensor for lens-free fluorescence microscopy. Lens-free imaging enables compact, low-cost systems with a large field-of-view ( $> 20$  mm) and pixel-limited resolution (1.4 micrometer). To overcome the limitations of conventional colour filters, in particular their strong angular dispersion, we integrate a polariton-based filter directly on the sensor. This novel filter design exploits ultra-strong light-matter coupling between photons and material excitons, maintaining a stable long-pass cut-off below 540 nm over a broad range of incidence angles and thereby drastically improving the signal-to-noise ratio. Initial results highlight the potential for high-resolution on-chip lens-free fluorescence microscopy with significantly enhanced image quality.

BP 14.40 Tue 18:00 P2

**Construction of Mueller Matrix Polarimeter with a Polarization Camera** — •KATHRIN ROTT — Georg August Universität, Göttingen, Deutschland

A Mueller matrix polarimeter based on a division-of-focal-plane polarization camera has been developed for microscopy. The setup enables spatially resolved measurements of Mueller matrix elements in a single image acquisition, allowing the extraction of polarization parameters such as retardance, diattenuation and depolarization. The setup includes a polarization state generator (PSG) consisting of a linear polarizer and a rotating compensator, and a polarization state analyzer (PSA) implemented through the micro-polarizer array of the camera. This design allows fast measurement of Mueller matrix images with micrometer-scale resolution. Initial work focused on characterizing the camera, including calibration of nonlinear response, sensor homogeneity, polarization angle accuracy and pixelwise extinction ratio. The aim is to enable label-free imaging of biological cell cultures and to investigate whether polarization-based contrast can provide information about microstructures such as the cytoskeleton or nucleus. Unlike tissue samples, which typically exhibit polarization effects, the focus here lies on exploring polarization contrast in single cells. The project combines optical component development with a potential biophysical application and forms the basis for further studies on polarization contrast in cell culture imaging.

BP 14.41 Tue 18:00 P2

**Quantification of in vivo flow of blood cells - adhesion cascade** — •KHADIJA LARHRISSI<sup>1</sup>, FELIX MAURER<sup>1</sup>, SELINA WRUBLEWSKY<sup>2</sup>, ALEXIS DARRAS<sup>3</sup>, and CHRISTIAN WAGNER<sup>1</sup> — <sup>1</sup>Department of Experimental Physics, University Campus, Saarland University, 66123 Saarbrücken, Germany. — <sup>2</sup>Institute for Clinical and Experimental Surgery, Saarland University, 66421 Homburg, Germany — <sup>3</sup>School of Physics, University of Bristol, Bristol, United Kingdom)

Red blood cells (RBCs) constitute the majority of cells in the blood and play a key role in transporting oxygen to tissues and organs. On the other hand, leukocytes, also known as white blood cells (WBCs), make up approximately 1% of the total blood volume in most mammals. The flow of these cells ensures the body's defense against various viral and bacterial infections. The WBCs exhibit two modes of motion: a fast flow mode where they move with the surrounding fluid, and a slower rolling mode where they partly adhere to the wall, whereas RBCs simply flow with the surrounding fluid. In this study, our objective is to examine the influence of geometry and distribution on the flow of WBCs. To achieve this, we used Golden Syrian Hamsters as a model system to quantify the flow of cells by fluorescence microscopy and compare their behavior in different networks of vessels. Additionally, since some WBCs are larger in size than the capillaries they pass through, we will examine the impact of this size difference on their flow.

BP 14.42 Tue 18:00 P2

**Visualizing Immune Cell Behaviour in 3D: An Ex Vivo Lattice Lighsheet Microscopy and Analysis Framework** — •ANNA SCHEPERS<sup>1</sup>, JOANNAH FERGUSSON<sup>1</sup>, EDWARD WHEELER<sup>1</sup>, JACKY KO<sup>1</sup>, ROBERT KOCHL<sup>2</sup>, and MARCO FRITZSCHE<sup>1</sup> — <sup>1</sup>Kennedy Institute of Rheumatology, University of Oxford, UK — <sup>2</sup>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 tech-

nological 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. We present a complex data processing and analysis framework for robust 3D segmentation and tracking cells in the complex tissue environment allowing cell profiling from live cell behaviour. 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.

BP 14.43 Tue 18:00 P2

**Large-area AFM SmartMapping for contact lens characterization and mechanobiological tissue analysis** — •JÖRG BARNER, ANDRE KÖRNIG, JOAN-CARLES ESCOLANO, and THOMAS HENZE — BioAFM, Bruker Nano Surfaces, Am Studio 2D, 12489 Berlin, Germany

Atomic force microscopy (AFM) provides quantitative nanoscale characterization of soft materials and biological systems, enabling analysis of surface topography, elasticity, and viscoelasticity under physiologically relevant conditions. We applied AFM to two distinct systems: ophthalmic contact lenses and highly corrugated tissues. For lenses, SmartMapping was used to acquire large-area curvature maps (up to several millimeters) combined with localized high-resolution measurements of nanomechanical properties. Silicone hydrogel lenses were analyzed, revealing heterogeneities in elasticity critical for balancing oxygen permeability and comfort. For biological samples, SmartMapping enabled automated imaging of rough, heterogeneous specimens such as 3D tumor spheroids ( $>100$  um) and brain tissue sections ( $>300$  um), capturing stiffness gradients relevant to mechanotransduction and transport. The synchronized XYZ-piezo and AFM head movement ensured reproducible mapping across extended areas without manual intervention, overcoming limitations of conventional AFM in lateral range and throughput. These results demonstrate that SmartMapping integrates large-scale imaging with nanoscale precision, establishing AFM as a robust platform for material optimization in ophthalmology and spatially resolved mechanobiological studies.

BP 14.44 Tue 18:00 P2

**X-ray holo-tomography reveals 3D structure of protein networks and lipid globules in heat-treated egg yolk** — •FELIX WITTWER<sup>1,2</sup>, NIMMI DAS ANTHUPARAMBIL<sup>2</sup>, FREDERIK UNGER<sup>2</sup>, RANDER PRATAP GAUTAM<sup>2</sup>, SILJA FLENNER<sup>3</sup>, IMKE GREVING<sup>3</sup>, CHRISTIAN GUTT<sup>2</sup>, and PETER MODREGGER<sup>1,2</sup> — <sup>1</sup>Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — <sup>2</sup>Universität Siegen, Siegen, Germany — <sup>3</sup>Helmholtz-Zentrum Hereon, Geesthacht, Germany

Egg yolk is a versatile ingredient for cooking and food processing. As a natural emulsifier, it allows to bind fats and water. Under heating, the texture and consistency of egg yolk changes due to denaturation, aggregation, coagulation and gelation. By using X-ray holo-tomography, we could study the heat-induced changes in egg yolk on the micron to sub-micron length scale. In contrast to other techniques such as electron microscopy, X-ray holography can be used without sample staining, fixation, or drying, which potentially alter or damage the sample. Our results reveal a developing separation between proteins and lipids with fatty components rapidly aggregating into large globules around 40 micrometer in size.

BP 14.45 Tue 18:00 P2

**Realignment and realization of polarization-resolved confocal FLIM** — •LIZHONG MOU<sup>1</sup>, SHANGJUN CHENG<sup>1,2</sup>, SUBHAM ADAK<sup>1,2</sup>, MARYAM ALI<sup>1,2</sup>, DANIELA TÄUBER<sup>1,2</sup>, and RAINER HEINTZMANN<sup>1,2</sup> — <sup>1</sup>Friedrich Schiller University Jena — <sup>2</sup>Leibniz Institute of Photonic Technology, Jena

Fluorescence lifetime imaging microscopy (FLIM) is an attractive technique in the life sciences that enables quantitative mapping of excited-state lifetimes in the regime of nanoseconds within microscopic images [Le Marois et al., J. Biophot. 2017, 10,1124]. Conventional fluorescence polarization is widely used to assess the orientation and rotation of molecules but typically relies on millisecond acquisition times [Camacho et al., Adv. Mat. 2019, 31, 1805671]. Here, we present an alignment protocol for polarization-resolved confocal FLIM that delivers nanosecond temporal resolution and high-quality imaging. We further investigate time-resolved polarization states of dye molecules

from cell and tissue samples.

BP 14.46 Tue 18:00 P2

**Physics Informed Neural Networks for Microbial Interaction Network Inference** — •LUCA BATTISTON<sup>1,2</sup> and FRANK CICHOS<sup>1</sup> — <sup>1</sup>Universität Leipzig, Linnestr. 5, 04103, Leipzig, Germany — <sup>2</sup>Helmholtz Centre for Environmental Research GmbH (UFZ), Permoserstr. 15, 04318, Leipzig, Germany

Recent advances in machine learning have enabled data-driven modeling of complex dynamical systems, with growing interest in methods that extract meaningful information about the underlying physical laws. Among these, Physics-Informed Neural Networks (PINNs) have emerged as a powerful tool for system identification, particularly in settings where data are scarce or noisy. On the other hand, generalized Lotka-Volterra (gLV) equations are widely used to model microbial community dynamics, provided that the underlying interaction matrix is known. In this work, we aim to reconstruct these interactions by combining PINNs with Least Squares Regression for inference of the interaction network. We evaluate our method using extensive gLV simulations covering a range of interaction matrix complexities and noise levels. Our results demonstrate high accuracy in network recovery and show that the approach retains robustness under measurement noise. This provides a step toward developing a robust and flexible framework for identification of complex interaction patterns in microbial communities.

BP 14.47 Tue 18:00 P2

**Experimental Setup for the Irradiation of Organoids with High-Energy Electron Beams** — •LAURA ANDREA PASTOR LUQUE<sup>1</sup>, NATASCHA THOMAS<sup>2</sup>, VICTOR EMDE<sup>2</sup>, CARLA SPRENGEL<sup>1</sup>, ANTONIO TARZIKHAN<sup>2</sup>, CONSTANTIN ANICULAESEI<sup>1</sup>, THOMAS HEINEMANN<sup>2</sup>, MIRELA CERCHEZ<sup>2</sup>, and THOMAS HEINZEL<sup>1</sup> — <sup>1</sup>Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — <sup>2</sup>Institut für Laser- und Plasmaphysik, Heinrich Heine University, Düsseldorf, Germany

Organoids are three-dimensional cell systems that mimic key physiological and structural characteristics of human tissues, making them highly relevant models for studying biological responses to ionizing radiation. However, experimental platforms for irradiating organoids with high-energy electron beams remain limited, particularly regarding precise dose control and sample handling. In this work, we present the design and development of an experimental irradiation setup specifically adapted for organoid cultures. The system integrates a high-energy electron beam source with a setup to irradiate organoids samples at different energy ranges (MeV).

BP 14.48 Tue 18:00 P2

**Evolution-inspired exploration of pattern formation in reaction diffusion systems** — •MING HONG LUI<sup>1,2</sup> and ERWIN FREY<sup>1,2</sup> — <sup>1</sup>Faculty of Physics, Ludwig Maximilian University of Munich, Germany — <sup>2</sup>Max Planck Schools Matter to Life, Max Planck Institute for Medical Research, Heidelberg, Germany

Protein reaction networks often contain complex network topology. Modelling them involves numerous variables such as concentrations, diffusion rates and kinetic coefficients. Each variable adds an additional dimension to the phase space that made sweeping parameters challenging and impedes comprehensive understanding of the full dynamics by demanding assumptions or simplifications of biological systems.

Here, we present an alternative pipeline to full parameter sweeps, to characterize pattern-forming regimes, by applying an evolutionary algorithm. We iteratively bootstrapped parameter combinations that demonstrated instability using linear stability analysis. Together with applying mutations, represented by random displacements on the high-dimensional phase space, we could focus our attention in the vicinity of instabilities to reconstruct a heuristic phase diagram more effective than evenly-spaced parameter sweeps.

We shall demonstrate how this algorithm can be applied to various reaction-diffusion models, where it provided more informed choices of diverse systems to run full numerical simulations on, bridging the gap between analytical and numerical solutions.

BP 14.49 Tue 18:00 P2

**Pancreatic Network Morphogenesis** — •YASMIN ABDELGHAFFAR<sup>1</sup>, COLINE SCHEWIN<sup>2</sup>, SZabolcs HORVÁT<sup>3</sup>, MONALISA MISHRA<sup>2</sup>, LYDIE FLASSE<sup>2</sup>, CARL MODES<sup>2,4</sup>, ANNE GRAPIN-BOTTON<sup>2</sup>, and BENJAMIN M. FRIEDRICH<sup>1,4</sup> — <sup>1</sup>Cluster of Excellence Physics

of Life, Technical University Dresden, Dresden, Germany — <sup>2</sup>Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — <sup>3</sup>Reykjavík University, Reykjavík, Iceland — <sup>4</sup>Center for Systems Biology Dresden, Dresden, Germany

During the course of development, the mammalian pancreatic ductal network remodels from a fully connected plexus to a tree-like branched network optimized for fluid transport. Previous *in silico* modeling suggested that this remodeling could be guided by flow through the network [1]. However, the physical mechanism of flow sensing in the developing pancreas remains open.

We quantitatively analyze duct network morphology at subsequent developmental time-points, to reverse-engineer putative physical mechanisms of network remodeling. This includes a spatial zonation of statistical network properties and an empirical Murray's law relating duct diameter to hierarchy level (Strahler number). We put forward theoretical descriptions, e.g., of cilia-based flow sensing, which reproduce distinct variants of Murray's law, which could be distinguished by future experiments.

[1] Dahl-Jesen et al., PLoS Biology, 2018.

BP 14.50 Tue 18:00 P2

**A Mathematical Model of Microlesion-Driven Calcium Signalling in Fibroblast Networks** — •KARA NACHTNEBEL<sup>1,2,3,5</sup>, ERIC GRETO<sup>1,2,3</sup>, ANNA MÖLLER<sup>1,2,3,6</sup>, CHRISTIAN MAUERÖDER<sup>1,2,3</sup>, DAVID B. BLUMENTHAL<sup>6</sup>, VASILY ZABURDAEV<sup>4,5</sup>, and STEFAN UDERHARDT<sup>1,2,3</sup> — <sup>1</sup>Department of Medicine 3 - Rheumatology and Immunology, FAU und Universitätsklinikum Erlangen — <sup>2</sup>Deutsches Zentrum für Immuntherapie, FAU — <sup>3</sup>Exploratory Research Unit, Optical Imaging Centre Erlangen, FAU — <sup>4</sup>Department of Biology, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) — <sup>5</sup>Max-Planck-Zentrum für Physik und Medizin, Erlangen — <sup>6</sup>Department of Artificial Intelligence in Biomedical Engineering, FAU, Erlangen, Germany

Resident tissue macrophages (RTMs) maintain tissue homeostasis by continuously sensing and integrating local environmental signals. The interstitial fibroblast network, an omnipresent, self-interconnected system capable of generating intracellular calcium signals and transmitting them to neighbouring cells, provides signals that RTMs can detect and respond to. For example, in response to calcium elevations associated with tissue lesions, macrophages initiate rapid cloaking behaviour. Disruption of fibroblast networks can amplify unwanted immune activation and may contribute to the development of autoimmune diseases. We present a mathematical model of microlesion-induced calcium signalling in gap-junction-coupled fibroblast networks. It shows how microlesions drive signal propagation via intra- and extracellular pathways and quantifies the factors that shape this process.

BP 14.51 Tue 18:00 P2

**Equal Partitioning of the Min Proteins at Cell Division** — •NATAN DOMINKO KOBILICA<sup>1</sup>, NORA DEIRINGER<sup>2</sup>, VITALII GRIGOREV<sup>3</sup>, ANTONIA WINTER<sup>1</sup>, ROBIN KÖHLER<sup>4</sup>, SEAN MURRAY<sup>5</sup>, VIKTOR SOURJIK<sup>3</sup>, HENRIK WEYER<sup>6</sup>, and ERWIN FREY<sup>1</sup> — <sup>1</sup>ASC, LMU München, Munich, Germany — <sup>2</sup>Technical University of Munich, Garching, Germany — <sup>3</sup>Max Planck Institute for Terrestrial Microbiology, Marburg, Germany — <sup>4</sup>Geomagic, Leipzig, Germany — <sup>5</sup>IMESO-IT, Giessen, Germany — <sup>6</sup>Kavli Institute for Theoretical Physics, University of California, Santa Barbara, Santa Barbara, USA

The pole-to-pole oscillation of the Min proteins in *Escherichia coli* plays a crucial role in the process of cell division. The oscillation facilitates the formation of the FtsZ ring, which determines the division site. It is essential that the Min proteins are distributed equally between daughter cells to ensure precise determination of the division site in subsequent divisions. Previously, experiments and stochastic particle-based simulations have linked protein equipartition to the splitting of the pole-to-pole oscillation. Importantly, the splitting is already triggered before the division is fully completed. The goal of this study is to explain the mechanism underlying the splitting of oscillations using the well-known reaction-diffusion equations for the Min System. We model the constriction during cell division as a reduced diffusion rate between the two parts of the mother cell. This already captures the oscillation splitting and agrees well with realistic simulations of the constricting cell. Additionally, we conduct high-throughput microfluidic experiments which align well with the predicted protein dynamics.

BP 14.52 Tue 18:00 P2

**Information Processing and Scaling of Spatially Coupled Complex Networks** — •AMBAR NEEL<sup>1,2,3</sup> and CARL MODES<sup>1,2,3</sup>

— <sup>1</sup>Max Planck Institute for Molecular Cell Biology and Genetics (MPI-CBG), Dresden 01307, Germany — <sup>2</sup>Center for Systems Biology Dresden (CSBD), Dresden 01307, Germany — <sup>3</sup>Cluster of Excellence, Physics of Life, TU Dresden, Dresden 01307, Germany

Biological adaptive spatial networks are constantly grappling with increasing the efficiency of the network while minimising the metabolic costs. Simulations demonstrate that incorporating fluctuations in a system's sinks/sources leads to the onset of topological complexity in the network. Additionally, it has recently been shown that coupling two spatial networks also results in topological complexity categorised by the existence of loops. This framework is very well suited to investigating information processing in such spatially coupled networks and is thus the focus of this presentation. Along with organ systems such as the pancreas, kidney and bone marrow, the liver is a prime candidate for this analysis as it consists of bile and blood capillary systems that are interwoven. Another challenge is to understand the packing limit of these complex spatial networks by scaling them until a critical point is reached. This provides a meaningful length-scale for the system, allowing for further investigation into fundamental questions regarding geometrical aspects of these spatially embedded complex networks as well as setting up the template to compare these results to experimentally acquired datasets of sinusoids in the liver lobules of mice.

BP 14.53 Tue 18:00 P2

**Chimeric RNA-DNA Oligomers Overcome Template-Product Inhibition in Prebiotic Ligation** — •LENA

MÜHLSCHLEGELE, LUDWIG BURGER, and ULRICH GERLAND — Physics of Complex Biosystems, School of Natural Sciences, Department of Bioscience, Technical University of Munich, Garching, Germany

The RNA world hypothesis proposes that DNA-based life evolved from a precursor living system that used RNA alone to store genetic information. However, it is unclear how the transition from a system purely based on RNA to one incorporating DNA could have occurred. At the transition, a lack of specificity in the synthesis of genetic polymers in prebiotic systems likely led to the simultaneous emergence of RNA and DNA, involving molecules comprising RNA-DNA nucleotides, which we refer to as chimeric RDNA strands. Because homogeneous RNA-RNA and DNA-DNA duplexes are highly stable, template-product inhibition can impede template-directed ligation. Experimental data show that RDNA-DNA or RDNA-RNA duplexes tend to be less stable than RNA-RNA and DNA-DNA duplexes, suggesting that RDNA strands might overcome template-product inhibition. We developed a nearest neighbor model parametrized by experimental data to predict RDNA hybridization energies as a function of sequence and used it to simulate template-directed ligation of RNA and DNA in the presence and absence of RDNA strands. We found a hybridization free energy regime in which RDNA strands enable the efficient replication of RNA and DNA, providing a potential pathway for the early evolutionary transition from RNA to DNA.

BP 14.54 Tue 18:00 P2

**FRET-guided selection of RNA 3D structures** — •MIRKO

WEBER<sup>1</sup>, FELIX ERICHSON<sup>1</sup>, MACIEJ ANTCZAK<sup>2,3</sup>, VANESSA SCHUMANN<sup>1</sup>, JOSEPHINE MEITZNER<sup>1</sup>, TOMASZ ZOK<sup>3</sup>, FABIO D. STEFFEN<sup>4</sup>, MARTA SZACHNIUK<sup>2,3</sup>, and RICHARD BÖRNER<sup>1</sup> —

<sup>1</sup>Laserinstitut Hochschule Mittweida, University of Applied Sciences Mittweida, Mittweida, Germany — <sup>2</sup>Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poznan, Poland — <sup>3</sup>Institute of Computing Science, Poznan University of Technology, Poznan, Poland — <sup>4</sup>Department of Oncology, University of Zurich, Zurich, Switzerland

Integrative RNA modeling requires structurally validated ensembles and experimental data that reflect binding and folding behavior. However, predicting such structure collections remains challenging due to rugged energy landscapes and extensive conformational heterogeneity. We address these limitations with a FRET-guided selection strategy that identifies RNA conformational states consistent with single-molecule FRET (smFRET) data. We predicted 3D structures of a ribosomal RNA tertiary contact containing a GAAA tetraloop and a kissing loop using RNAComposer, FARFAR2, and AlphaFold3, and validated them based on Watson-Crick base pairing and an eRMSD threshold. For all retained models, we computed accessible contact volumes of the sCy3/sCy5 dye pair using FRETraj and derived FRET distributions, which were weighted against experimental smFRET data. Our results demonstrate that *in silico* predicted structures can reproduce the experimental transfer efficiencies, and that our selection reliably identifies RNA conformations consistent with the smFRET data.

BP 14.55 Tue 18:00 P2

**Intrinsically disordered regulators of endocytosis - an integrated NMR/single molecule fluorescence approach** — •SIGRID MILLES — Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany

Intrinsically disordered proteins (IDPs) lack clearly defined structure and are therefore highly flexible and easily adaptable to different binding partners. This makes them important players in many biological processes, often with vital regulatory functions. Their dynamic features and broad range of interaction modes, however, render them difficult to study and analyzing their complexes often requires integrated approaches. Integrating complementary parameters from of nuclear magnetic resonance (NMR) and single molecule fluorescence approaches allowed us to describe the conformational landscape of IDPs at molecular resolution and promises to shed new light onto various biological processes. Among those counts clathrin mediated endocytosis. The early phases of clathrin mediated endocytosis are organized through a highly complex interaction network mediated by clathrin associated sorting proteins (CLASPs) that comprise long intrinsically disordered regions (IDRs). We characterize the IDRs of those CLASPs in their entirety and at molecular resolution, uncovering a plethora of interactions of various strengths and dynamic features with their endocytic interaction partners, proposing a rationale for how first interactions and dynamic rearrangement of partners take place during the uptake of a coated vesicle.

BP 14.56 Tue 18:00 P2

**Adaptive NK cell analysis by t-SNE** — •ANDREA SCHNEIDER<sup>1</sup>,

WIEBKE MOSKORZ<sup>2</sup>, JÖRG TIMM<sup>2</sup>, and THOMAS HEINZEL<sup>1</sup> —

<sup>1</sup>Heinrich-Heine University Duesseldorf — <sup>2</sup>University Hospital of Duesseldorf

High-dimensional flow cytometry data from Natural Killer (NK) cells, collected using a comprehensive panel of typical and adaptive NK cell markers, poses a challenge for the characterization of complex cell subsets. To visualize the complete receptor expression profile in a two-dimensional cellular plot, we applied t-distributed Stochastic Neighbor Embedding (t-SNE) to the multi-parameter dataset. The resulting t-SNE projection successfully resolved distinct immune subpopulations regarding NK cell development and adaptive NK cells. Crucially, the map enabled the simultaneous visualization and comparison of different definitions of adaptive NK cells (including NKG2C+ and FcεRIg<sup>+</sup> subsets within mature NK cells), visually confirming their close relatedness. Furthermore, while CD95 is known to be increased in adaptive NK cells, the t-SNE visualization clearly confirmed that this high expression level is consistently shared across all defined adaptive cell clusters, which were tightly localized within the embedding. This methodology demonstrates the power of non-linear embedding techniques for validating complex immunological phenotypes. Moreover, it establishes a visual framework for comparative studies of NK cells across different patient groups, including Hepatitis C Virus (HCV) seronegative, chronically HCV infected, and HCV resolved donors, with each cohort further stratified by Cytomegalovirus serostatus.

BP 14.57 Tue 18:00 P2

**Exploring coarse graining RNA force fields via Machine Learning** — •ANTON EMIL DORN<sup>1</sup>, EMILE DE BRUYN<sup>1</sup>, FABRICE

VON DER LEHR<sup>3</sup>, STEFAN KESSELHEIM<sup>1,4</sup>, PHILIPP KNECHTGES<sup>3</sup>, and

ALEXANDER SCHUG<sup>2</sup> — <sup>1</sup>Forschungszentrum Jülich — <sup>2</sup>KIT — <sup>3</sup>DLR

Köln — <sup>4</sup>Universität zu Köln

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 to 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. We also explore different bead numbers for the coarse graining to determine the best approximation.

BP 14.58 Tue 18:00 P2

**Segmentation and classification of retinal pigment organelles in fluorescence lifetime imaging microscopy (FLIM) data** — •MARYAM ALI<sup>1,2</sup>, HALA ALHAJ AHMED<sup>3,4</sup>, MARTIN HAMMER<sup>4</sup>,

RAINER HEINTZMANN<sup>1,2,5</sup>, and ONDREJ STRANIK<sup>1,2</sup> — <sup>1</sup>Leibniz Institute of Photonic Technology, Jena, Germany — <sup>2</sup>Friedrich Schiller University, Jena, Germany — <sup>3</sup>Ernst-Abbe University of Applied Sci-

ences, Jena, Germany — <sup>4</sup>Jena University Hospital, Jena, Germany — <sup>5</sup>Abbe Centre of Photonics, Jena, Germany

Retinal Pigment Epithelium (RPE) granules can be categorized based on their autofluorescence and morphology like Lipofuscin (L), Melanolipofuscin (ML), and Melanin(M)[1]. Fluorescence lifetime measurements reveal another discriminative feature; however, identifying individual granules remain challenging by human eye. Here, we present a computational analysis pipeline for segmenting and classifying RPE granules from fluorescence lifetime imaging microscopy (FLIM) data. The analysis was implemented in a custom Python script employing seeded watershed segmentation to isolate individual granules and discriminate hyperfluorescent lipofuscins, characterized by longer lifetimes. Granules with shorter lifetimes were further analyzed by examining their lifetime distribution across their surfaces, allowing MLs to be distinguished from other melanin-rich granules. The proposed approach achieved high performance, with mean sensitivity 87% and mean specificity 98% compared to manually classified ground truth data. [1] K. Bermond et al., IOVS 2020, 61, 35

BP 14.59 Tue 18:00 P2

**Modeling the Clustering of Pma1 in the Yeast Plasma Membrane under Starvation** — •ANNEMARIE QUAS<sup>1</sup>, ROLAND WEDLICH-SÖLDNER<sup>2</sup>, and ANDREAS HEUER<sup>1</sup> — <sup>1</sup>Institut für Physikalische Chemie, Universität Münster — <sup>2</sup>Institut für Zelldynamik und Bildgebung, Universität Münster

Starvation of yeast cells leads to the internalization of most plasma membrane (PM) proteins via endocytosis, strongly reducing the overall protein content of the PM. However, the level of the H<sup>+</sup>-ATPase Pma1 is hardly affected by starvation. Instead, clustering of Pma1 is observed under these conditions. FF-EM images reveal 2D crystals composed of hexagonal units corresponding to Pma1 hexamers. Interestingly, deletion of Mrh1 blocks the clustering of Pma1. An interplay between the positively charged C-terminus of Mrh1 and the negatively charged phosphatidylserine (PS) is proposed, as Mrh1 is not required for clustering in the absence of PS. Because experimental insight into the mechanism of cluster formation is limited, we employ a coarse-grained Monte-Carlo model to investigate how interactions between Pma1 hexamers can drive large-scale organization. In our 2D model, Pma1 is represented as hexamers with attractive corner-to-corner interactions. By systematically varying particle density and interaction strength, we explore the system's phase behavior and identify conditions under which extended cluster formation emerges. We analyze cluster sizes, time-dependent growth, and characteristic cluster shapes to gain mechanistic insight into how molecular interactions could stabilize the observed protein crystals.

BP 14.60 Tue 18:00 P2

**Refining Coarse-Grained Models for Accurate Protein Folding and Mechanics** — •YI-CHEN TSAI and CHI-CHENG CHIU — National Cheng Kung University, Tainan, Taiwan

Accurately modeling protein folding and mechanical behavior in coarse-grained (CG) simulations requires balancing structural fidelity with physical realism. We develop a mesoscale modeling framework that advances CG protein simulations by integrating refined structure-based and hybrid physics-based approaches. The Gō-type structure-based model is refined by incorporating overlaid native-specific potentials, backbone dihedrals, improper torsions, and sidechain interactions. These additions improve folding accuracy, suppress chiral inversion, and yield more realistic mechanical responses across diverse proteins[1]. Building on this, a hybrid CG approach denoted as GoSPICA is developed by combining native-contact potentials with the physics-based SPICA CG force field. The hybrid model enables spontaneous folding, reproduces native fluctuation patterns and force-extension behavior, and remains fully compatible with membrane environments without relying on elastic network restraints. Together, these developments establish a versatile CG modeling framework for simulating protein behavior in biologically relevant environments.

[1] Y. Tsai et al., *Phys. Chem. Chem. Phys.*, Advance Article (2025).

BP 14.61 Tue 18:00 P2

**PINNs based inference in reaction-diffusion systems** — •LUKAS PÖSCHL<sup>1,2</sup> and VASILY ZABURDAEV<sup>1,2</sup> — <sup>1</sup>Friedrich-Alexander Universität Erlangen-Nürnberg — <sup>2</sup>Max Planck Zentrum für Physik und Medizin

Physics-informed neural networks (PINNs) promise to serve as uni-

versal function approximators that embed governing equations and biophysical constraints to operate under noisy, low data conditions. However, PINNs exhibit various training pathologies that limit broad practical application beyond simple benchmarking problems. We identify situations in biophysical models where PINNs fail, including stiff kinetics, sharp gradients and chaotic dynamics and map these to corresponding failure modes in the standard PINN formulation, together with the respective mitigations. We assess this improved formulation on four problems with synthetically generated experimental data. These tasks include the classical forward and inverse problems for parameter estimation and inference of experimentally inaccessible species. Furthermore, we address the issue of discovering chaotic and pattern forming dynamics and thus the optimization of experimental parameters to explore these biophysically relevant regimes. Across selected problems, the modified PINNs suggest promising performance in handling the tested systems and the ability to operate with sparse measurements and noisy data.

BP 14.62 Tue 18:00 P2

**Self-assembly of sarcomeres by pairwise interactions in muscle fibers** — •AMIRALI ZANDIEH, ABHINAV KUMAR, FRANCINE KOLLEY-KÖCHEL, and BENJAMIN M. FRIEDRICH — Cluster of Excellence "Physics of Life", Dresden University of Technology

Walking, flying, and heartbeat are powered by the contraction of sarcomeres, the elementary contractile units of striated muscle, which are arranged in series into periodic myofibrils extending across the length of a muscle cell [1]. While the physical principles underlying sarcomere self-assembly remain unclear, recent work on *Drosophila* indirect flight muscle revealed that myosin motor filaments, Z-disk proteins, and titin/Sallimus form an initial periodic pattern, with actin filaments becoming polarity-sorted only later, motivating 1D minimal models [2].

To develop more realistic 3D descriptions of myofibrillogenesis and capture their cross-sectional organization, we employ ESPResSo [3] for agent-based simulations. With only pairwise interactions, sarcomere-like periodic patterns emerge and become registered in-phase along the transverse direction, as quantified by Kuramoto order parameters. Additionally, the catch-bond behavior of actin crosslinkers enhances and stabilizes this order. Together, these results show that pairwise interactions between sarcomeric components are sufficient to drive the emergence of order, marking a key step toward understanding the physical basis of sarcomere self-assembly.

[1] F. Kolley, et al. *PRX Life* (2024) [2] F. Kolley-Köchel, et al. *Biophysical Reviews*, in press [3] Weik, Florian, et al. *The European Physical Journal* (2019)

BP 14.63 Tue 18:00 P2

**Assessing the performance of quantum-mechanical descriptors in physicochemical and biological property prediction** — •ALEJANDRA HINOSTROZA CALDAS<sup>1</sup>, ARTEM KOKORIN<sup>2</sup>, ALEXANDRE TKATCHENKO<sup>2</sup>, and LEONARDO MEDRANO SANDONAS<sup>1</sup> — <sup>1</sup>TUD Dresden University of Technology, 01069 Dresden, Germany — <sup>2</sup>University of Luxembourg, L-1511 Luxembourg City, Luxembourg

Understanding how molecular structure relates to physicochemical and biological properties is essential for computer-aided drug design. A major challenge in applying machine learning (ML) to this problem is defining numerical representations that capture both geometric and electronic information. We introduce the QUantum Electronic Descriptor (QUED) framework [ChemRxiv, doi:10.26434/chemrxiv-2025-hj4dc], which integrates geometric descriptors (BOB, SLATM) with a quantum-mechanical descriptor ( $D_{QM}$ ) that encodes global and local electronic properties computed efficiently with the DFTB method. We validate QUED on the QM7-X dataset of small drug-like molecules and show that incorporating electronic structure information substantially improves ML predictions of physicochemical properties. For biological endpoints, QUED also demonstrates predictive value for acute toxicity (LD50) in TDCommons-LD50 and for lipophilicity in the MoleculeNet benchmark. Our findings underscore the benefits of integrating electronic structure information with geometric descriptors and highlight the role of conformational diversity in improving the robustness of molecular property prediction.

BP 14.64 Tue 18:00 P2

**Modelling neuron growth dynamics and role of extra-cellular matrix** — •MATHAR KRAVIKASS, FEDERICA FURLANETTO, LARS BISCHOF, PRITHA DOLAY, BEN FABRY, SVEN FALK, MARISA KAROW, and VASILY ZABURDAEV — Friedrich-Alexander-Universität (FAU)

Biological tissues are composed of cells embedded in extracellular ma-

trix (ECM) and extracellular fluid. We study the role of cell-matrix interactions in the context of brain tissues and the mechanism of neurite 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 modeled ECM particles. In a liquid-like ECM model, we demonstrate how growth is influenced by the ECM interactions when the matrix is freely deformable. These growth patterns were also shown to fit to a run-and-tumble process, which describes how the interaction parameters relate to the persistence and speed of the growth. Additionally, solid-like ECMs were considered in which the ECM particles are connected by springs, thus forming a lattice. In this scheme, we were able to study more closely how lattice stiffness affects neurite growth patterns. These simulations recapitulated growth patterns of neurites in organoids models of neurodevelopmental disease and neurite growth in artificial ECMs with controlled properties. Finally, we present how this model could be used in the future to describe more complex systems, such as neuronal network formation.

BP 14.65 Tue 18:00 P2

**Motion or Player? Identifying Structural Drivers of Rare Transitions** — •ALI SHARIFIAN and ALEXANDER SCHUG — Scientific Computing Centre, Karlsruhe Institute of Technology, Karlsruhe, Germany

Rare transitions in complex molecular and soft-matter systems are often described by low-dimensional collective variables (CVs) that track progress between long-lived states. Here we distinguish between the motion -pathway in high-dimensional space- and the players -specific atoms, residues, or coarse-grained units- that most strongly drive that motion. With accurate structure prediction now routine for many proteins, the central challenge is to move from static models to a mechanistic view of functional dynamics based on full ensembles. We present an ensemble-based framework that takes high-dimensional structural data from simulations or experiments and, for any chosen CVs, identifies these structural players. From a structural ensemble and user-defined CVs, we construct the free-energy landscape, determine a minimum-barrier path between metastable states, and define a transition tube that isolates barrier-crossing configurations. Within this tube, a path-conditioned principal component analysis captures transition-specific fluctuations, while time-lagged independent component analysis resolves the associated slow modes. Combining each feature's contribution to variance and slowness into a single importance score yields a ranked map of transition hotspots. These hotspots can guide mutations, targeted coarse-graining, and allosteric drug design across biomolecular and synthetic systems.

BP 14.66 Tue 18:00 P2

**Electronic and structural properties of (doped) bilayer systems of graphene and molybdenene** — •SABRINA SMID — RWTH Aachen, Worringer Weg 3, 52074 Aachen

Two-dimensional (2D) materials have attracted intense interest since the discovery of semi-metallic graphene in 2004. Owing to its exceptional electronic, thermal, and mechanical properties, graphene has become a key platform for exploring van der Waals (vdW) heterostructures. Stacking different 2D crystals enables emergent phenomena absent in the isolated layers, as exemplified by graphene encapsulated in hexagonal boron nitride, where interfacial screening enhances carrier mobility. The introduction of twist angles in such heterostructures has further unlocked new electronic behavior, including flat-band correlated states in twisted bilayer graphene.

Recently, the emergence of metallic molybdenene, synthesized via microwave-assisted exfoliation of MoS<sub>2</sub>, has further expanded the 2D materials landscape. Its intrinsic metallic character and tunable properties in vdW architectures suggest promising opportunities for heterostructure engineering. Motivated by this, we additionally perform density-functional theory calculations on a vdW bilayer composed of semi-metallic graphene and metallic molybdenene, examining how twist angle and carrier doping modify its structural and electronic properties.

BP 14.67 Tue 18:00 P2

**Dynamic Generation of Rigidity and Curvature during Clathrin-mediated Endocytosis** — •JOHANNES DRECKHOFF, LEON LETTERMANN, and ULRICH SCHWARZ — University of Heidelberg, Germany

Clathrin-mediated endocytosis is a main transport pathway across cell membranes, yet the physical mechanisms by which the clathrin coat

assembles to drive generation of membrane curvature are not understood well. In particular, it has been argued that bending would not be possible if the coat attained its high stiffness already at the initial stages. Here we address this crucial issue using agent-based kinetic Monte Carlo simulations for coat assembly in spherical geometries with variable curvature. By formulating a microscopic Hamiltonian governing individual clathrin legs, we elucidate the interplay between lattice growth, topological defects, effective membrane stiffness and macroscopic curvature generation. Our simulations reveal that the effective bending rigidity of the coat increases by approximately two orders of magnitude during assembly, driving the curvature generation. We also observed the growth curvature imprinting itself onto the system, resulting in a "curvature memory" effect. Crucially, our simulations capture the distinct dynamical regimes observed in experiments: we successfully reproduce the flat-to-curved transition, while also predicting stalled, flat growth events, potentially driven by premature lattice stiffening. This unifying description demonstrates that clathrin-mediated endocytosis is a multi-faceted process during which rigidity and curvature are generated in a cooperative manner.

BP 14.68 Tue 18:00 P2

**Revealing Temporal Hierachy in Larval Zebrafish Behaviour and Its Neuronal Representation** — •LEONARD CONSTIEN<sup>1</sup>, GAUTAM SRIDHAR<sup>2</sup>, JOAO C. MARQUES<sup>3</sup>, DREW N. ROBSON<sup>3</sup>, JENNIFER M. LI<sup>3</sup>, ANTONIO C. COSTA<sup>1</sup>, and CLAIRE WYART<sup>1</sup> — <sup>1</sup>Paris Brain Institute (Institut du Cerveau), Sorbonne University, INSERM U1127, CNRS UMR 7225, Paris, France — <sup>2</sup>Okinawa Institute of Science and Technology 1919-1 Tancha, Onna-son, Kunigami-gun Okinawa, Japan 904-0495 — <sup>3</sup>Max-Planck-Institut für biologische Kybernetik, Tübingen, Germany

On a given timescale, animal behaviour can be structured into behavioural states, each defined by a similarity of kinematics, immediate goals and physiological states. Further, coarse behavioural state divide into substates, unfolding on faster timescales. How are these states represented in the brain and which structures control their dynamics across timescales? To address these questions, we apply a Markov chain analysis framework to a dataset of larval zebrafish behaviour with parallel recording of whole-brain activity at cellular resolution. The approach identifies behavioural states in a principled and unbiased manner and reveals a hierarchical organization of hunting behaviour from the seconds to minutes timescale. Further, by applying the framework independently on neuronal activity, we reveal a similar structure of the dynamics, identify representing brain regions and investigate the links to behaviour. This work will motivate further studies to determine the circuits and mechanisms behind the regulation of behavioural dynamics.

BP 14.69 Tue 18:00 P2

**Dynamic Health Monitoring: Predicting COVID-19 with Wearable Sensor Data and catch22 Features** — •PAUL BUTTKUS and DIRK BROCKMANN — Technical University Dresden (SynoSys), Dresden, Germany

In the initial stages of a pandemic, when intervention leverage is highest, controlling infectious-disease spread hinges on timely detection of emerging cases. The rapid, global transmission of COVID-19 highlighted the need for scalable sensing tools that can pick up early physiological signatures of infection. Using data from the Corona Data Donation Project, which provides resting heart rate, step count, and sleep duration time series from over 120,000 voluntary participants in uncontrolled, real-world settings, we trained regression models to classify COVID-19 test results. Based solely on daily aggregated features, this model achieved an above random guessing success rate, revealing a non-trivial signal despite coarse temporal resolution and strong noise. To better highlight the underlying dynamics, we employ the catch22 (22 Canonical Time-series Characteristics) feature set to map raw sensor data to a compact set of interpretable descriptors, and additionally extend our framework to higher-temporal-resolution data to incorporate periodicity metrics (e.g., circadian modulation of heart rate and activity) that are lost under daily aggregation. We show which dynamical features are most informative for distinguishing COVID-19-positive from negative individuals and discuss how this framework could turn large-scale wearable data into a real-time surveillance tool for public health.

BP 14.70 Tue 18:00 P2

**A Computational Approach to Drug Screening for the Sphingosine-1-Phosphate Receptor Family for Therapeutic**

**Use against Autoimmune Diseases** — •JANOS HINTZE, TIM BENNET HAUSMANN, JONATHAN HUNGERLAND, and ILIA SOLOV'YOV — Institute of Physics, Carl von Ossietzky Universität, Carl-von-Ossietzky-Str. 9-11, 26129 Oldenburg, Germany

Current drugs used in the treatment of multiple sclerosis (MS) often lead to a variety of unwanted side effects. Some of the target proteins in MS treatment are sphingosine-1-phosphate receptors (S1PRs), which form a family of five structurally similar G protein-coupled receptors (GPCRs) that are found in various tissues throughout the human body. In this work, a generative diffusion model was used to design a broad spectrum of novel ligand candidates. To account for receptor flexibility, molecular docking was performed on different protein conformations obtained through molecular dynamics (MD) simulations. Analysis of the generated ligand candidates showed a consistently low similarity to existing S1PR-targeting drugs. Approximately 2000 candidates show a favorable binding affinity and subtype-specific selectivity based on their docking scores. This dataset can be further investigated based on other criteria such as toxicity, synthesizability, and stability, aiming to identify selective ligands for S1PRs, relevant for MS therapy.

BP 14.71 Tue 18:00 P2

**Applying a topology sensitive metric for RNA contact prediction** — •CHRISTIAN FABER<sup>1</sup>, UTKARSH UPADHYAY<sup>1</sup>, OSKAR TAUBERT<sup>2</sup>, and ALEXANDER SCHUG<sup>1,2</sup> — <sup>1</sup>Jülich Supercomputing Centre, Forschungszentrum Jülich, 52428, Jülich, — <sup>2</sup>Scientific Computing Centre, Karlsruhe Institute of Technology, 76344, Eggenstein-Leopoldshafen

Predicting the spatial structure of non-coding RNA (*ncRNA*) is an important task for understanding fundamental processes in living nature. Physical force fields are used to infer the structure from a sequence using simulations on high-performance computers. However, the best results are obtained by incorporating probable contacts as additional restraints. These can be derived from evolutionary data using statistical methods or from more recent artificial intelligence (AI) algorithms.

In the past, the focus was on achieving the highest possible proportion of correctly predicted contacts, while the distribution of these contacts on the contact map was overlooked. We have demonstrated the importance of this distribution for structure prediction and have therefore introduced a measure of it.

In our current work, we apply our new metric to a state-of-the-art algorithm *Barnacle*. To achieve this, the algorithms must undergo complete retraining and a new dataset must be generated that avoids data leakage. While our results demonstrate the practical application of such a procedure, they also underscore the challenges posed by the limited availability of data for RNA molecules, a problem which becomes particularly apparent when modelling AI networks.

BP 14.72 Tue 18:00 P2

**Structure and Dynamics of Network-Forming Protein Solutions using SAXS and megahertz XPCS** — •ADRIAN MAXIMILIAN RODA LENTZ<sup>1</sup>, MICHAEL PAULUS<sup>1</sup>, MICHELLE DARGASZ<sup>2</sup>, FLORIAN WIELAND<sup>3</sup>, and CHRISTIAN GUTT<sup>2</sup> —

<sup>1</sup>Department Physics/DELTA, TU Dortmund, Dortmund, Germany

— <sup>2</sup>Department of Physics, University of Siegen, Siegen, Germany

— <sup>3</sup>Institute of Metallic Biomaterials, Helmholtz-Zentrum Hereon, Geesthacht, Germany

This study explores the structure of networks formed by the biopolymer hyaluronic acid, together with the dynamics of embedded proteins, in this framework ferritin and apoferritin. Hyaluronic acid is a major constituent of synovial fluid and a key component in tissue dynamics and repair; therefore, characterization is essential for advancing biomedical applications. Static Small-Angle X-ray Scattering (SAXS) conducted at P10 (DESY) and BL2 (DELTA) was employed for structural characterization, complemented by megahertz X-ray Photon Correlation Spectroscopy (XPCS) at MID (EuXFEL) to quantify the dynamics. First results indicate a pronounced impact of hyaluronic acid on the collective diffusion behavior of proteins.

BP 14.73 Tue 18:00 P2

**Quantum mechanical/molecular mechanics (QM/MM) calculations for absorption spectra of photoactive proteins, including many-body screening contributions** — •JELENA SCHMITZ<sup>1,2</sup>, MAXIMILIAN GRAML<sup>1,2</sup>, TILL RUDACK<sup>1,3</sup>, and JAN WILHELM<sup>1,2</sup> —

<sup>1</sup>Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Germany — <sup>2</sup>Institute of Theoretical Physics, University of Regensburg, Germany — <sup>3</sup>Structural Bioinformatics, Regensburg Center for Biochemistry, University of Regensburg, Germany

The GW method and the Bethe-Salpeter equation (BSE) capture many-body screening effects, important for the full quantum mechanical description of excitations in large biological structures. Spectral shifts in photoactive proteins resulting from conformational changes can be described using a hybrid quantum mechanics/molecular mechanics (QM/MM) framework [1]. Our work investigates the impact of incorporating GW+BSE in QM/MM calculations, and examines how larger QM regions influence the accuracy of predicted shifts. We aim to compare to experimental results and QM/MM calculations using different ab initio approaches [1]. In order to perform calculations on larger, non-periodic systems, we are implementing RI-DFT as a pre-calculation method within the CP2K software package, prior to GW. This could provide us with access significantly larger system sizes, even full electrostatic protein surroundings, and therefore even higher accuracies.

[1] ChemBioChem 20, 1766 (2019)

BP 14.74 Tue 18:00 P2

**Investigating molecular mechanisms of signaling in the multistep phosphorelay system of *Magnaporthe oryzae* via All-Atom Molecular Dynamics Simulations** — •JONAS PAULUS<sup>1</sup>, DENNIS MARTIN<sup>1</sup>, ANTONIA PREUSS<sup>1</sup>, MILENA RUNGE<sup>2</sup>, STEFAN JACOB<sup>2</sup>, and LUKAS STELZL<sup>1</sup> — <sup>1</sup>Institut für molekulare Physiologie, Mainz, Germany — <sup>2</sup>Institut für Biotechnologie und Wirkstoff-Forschung, Mainz, Germany

Pathogenic fungi cause an annual loss of 15% of the world's major crops and the phenylpyrrole class of fungicides are upon the most successful to combat these pathogens, precisely because of their specificity and outstanding resistance management. The mode of action (MoA) takes place in a multistep phosphorelay system (MSP) thereby hyperactivating the high osmolarity glycerol (HOG) signaling pathway, but has not yet been clarified in detail on molecular level. Using all-atom molecular dynamics (MD) simulations, we investigate the structural and functional mechanisms of the cytosolic osmosensor MoHik1, its phosphotransfer signaling cascade, and nuclear import of downstream effectors. With this, we aim to design a multidimensional model of signal encryption and fungicide action in fungal MSP systems which will provide both, fundamental insights into fungal signal transduction and the chance to shed light on MSP systems as target for antifungal strategies.

BP 14.75 Tue 18:00 P2

**Cryogenic Structural Stability of Human Serum Albumin in Aqueous Solution Studied by SAXS/WAXS** — •LUKAS TEPFER, MICHAEL PAULUS, JAQUELINE SAVELKOULS, and METIN TOLAN — TU Dortmund, Maria-Goeppert-Mayer-Straße 2, 44227 Dortmund

The behavior of proteins during extreme temperature changes plays a crucial role in the development of stable biopharmaceutical formulations. Freezing and thawing processes are widely used in the production, processing, and long-term storage of protein-based drugs, but they can cause denaturation, aggregation, or loss of biological activity.

Cryoprotectants such as glycerol or other polyols are commonly used to mitigate these effects. They can stabilize proteins and prevent aggregation, among other things by changing the water structure and the hydration shell.

For structural characterization of these processes, Small- and Wide-Angle X-ray Scattering offer direct access to protein conformation, intermolecular distances, and mesoscale ordering phenomena, enabling analysis of proteins in solution without crystallization.

In this work, we use SAXS/WAXS at beamlines BL2 and BL9 at DELTA to study human serum albumin in aqueous and cryoprotective environments during cooling down to  $-100^{\circ}\text{C}$  and subsequent thawing. This allows us to analyze structural changes, stability, and possible reorganization processes across the entire cryogenic temperature range.

BP 14.76 Tue 18:00 P2

**Coarse grained simulations for the peptide lge1 1-80** — AGAYA JOHNSON<sup>1</sup>, ANTON POLYANSKY<sup>2</sup>, TERPSICHORI ALEXIOU<sup>1</sup>, BOJAN ZAGROVIC<sup>2</sup>, and •SOFIA KANTOROVICH<sup>1</sup> — <sup>1</sup>Computational and Soft Matter Physics, University of Vienna, Kollingasse 14-16, 1090 Vienna

— <sup>2</sup>Department of Structural and Computational Biology, Campus-Vienna-Bio Centre 5, 1030, Vienna

Due to the structural heterogeneity and fast dynamics of the bimolecular condensates, capturing their organization requires a coarse-grained modeling approach that bridges atomistic details with mesoscale properties. In this work, we develop a coarse-grained model based on atom-

istic potentials to study the formation of condensates of Lge1, a protein of interest in biomolecular phase separation. We implemented non-bonded interactions for these peptides derived from iterative Boltzmann inversion, with Martini force field parameters and votca tool kit into the espresso simulation package. We employ cluster analysis as a criterion to ensure that all these CG models retain key features of the self-assembly and phase separation comparatively, as it is observed in atomistic simulations. By leveraging CG modeling, we extend simulations to longer timescales and larger system sizes, enabling us to explore whether biomolecular condensates form through phase separation, self-assembly, or aggregation. Our approach provides insights into the structural transitions of Lge1 within condensates and the fundamental mechanisms governing these transitions. This work contributes to the development of predictive models for biomolecular organization in crowded cellular environments.

BP 14.77 Tue 18:00 P2

**Investigating the binding of clients to small heat shock protein 16.5 using electrospray ion beam deposition and cryogenic electron microscopy** — •MANAMI IMADA, NOOR NASEEB, and STEPHAN RAUSCHENBACH — University of Oxford, Oxford, UK  
Small heat shock proteins (sHSP) act as the first line of defence, preventing protein aggregation. sHSP do this by binding to the protein under stress to form a stable complex. We explore how these sHSPs bind to clients such as lysozymes using cryogenic electron microscopy (cryo-EM). However, sHSP are hard to image due to their dynamic nature and potential to form different oligomers.

Electrospray ion beam deposition (ES-IBD) is used to deposit the sample onto the cryo-EM grids. ES-IBD utilises native mass spectrometry (nMS), which transfers the complexes into the gas phase intactly and allows for mass filtration of the ion beam by a quadrupole. This allows specific complexes and binding stoichiometries to be deposited selectively onto the cryo-EM grids to be imaged.

BP 14.78 Tue 18:00 P2

**Sparse sampling in single molecule spectroscopy** — •SEBASTIAN STADLER and MARKUS LIPPITZ — Universitätsstraße 30, 95447 Bayreuth

Single-molecule spectroscopy (SMS) is fundamentally limited by photobleaching, leaving only a short time window to record spectra from individual emitters. These constraints motivate measurement strategies that extract maximal information from minimal data. Sparse sampling provides a compelling alternative to traditional Fourier spectroscopy, which requires dense, uniformly spaced measurements to satisfy the Nyquist condition. In contrast to traditional Fourier spectroscopy, sparse or sub-Nyquist sampling enables accurate spectral reconstruction from substantially reduced datasets.

In this theoretical study, we explore optimized sparse sampling strategies using simulated single-molecule spectra. By systematically varying sampling patterns, we identify regimes and procedures in which sparse acquisition offers significant gains in efficiency without compromising spectral fidelity. As a conceptual example of such optimized strategies, we discuss the pathway toward sampling optimization based on ensemble spectra and adaptive sampling approaches that iteratively adjust measurement points based on previously obtained information.

Our results outline design principles for efficient measurement protocols and highlight the potential of sparse acquisition to push SMS beyond traditional limits imposed by photobleaching and limited interrogation time.

BP 14.79 Tue 18:00 P2

**Single-molecule PIE-FRET and nsFCS Studies of Metal Ion-dependent Folding of an rRNA Tertiary Contact** — •MARA HENSCHEL<sup>1</sup>, VANESSA SCHUMANN<sup>1</sup>, ANDREAS HARTMANN<sup>2</sup>, MICHAEL SCHLIERF<sup>2</sup>, and RICHARD BÖRNER<sup>1</sup> — <sup>1</sup>Laserinstitut Hochschule Mittweida, Mittweida, Germany — <sup>2</sup>Technische Universität Dresden, Dresden, Germany

Tertiary interactions in ribosomal RNA are crucial for shaping the folding landscape. However, the dynamics of these interactions across different timescales are not well understood. We investigate the tertiary contact of a double fluorescent-labelled ribosomal RNA from *Saccharomyces cerevisiae* at the single-molecule level *in vitro*. We quantify metal-ion-dependent folding and dynamics during K(I) and Mg(II) titrations using single-molecule PIE-FRET as a nanometre-distance readout combined with nanosecond fluorescence correlation spectroscopy (nsFCS). FRET-histograms reveals ion-dependent broadening beyond shot noise, indicating structural dynamics on the mi-

crosecond to millisecond timescale. Furthermore, nsFCS measurements show fast domain motions ranging from nanoseconds to microseconds. By employing two complementary labeling schemes, we distinguish local folding of the kissing loop from formation of the long-range tertiary contact, resolving distinct folding trajectories within the same RNA construct. Our results provide a dynamic insight of rRNA tertiary-contact formation and lay the foundation for a quantitative, mechanistic model of metal-ion-regulated folding of ribosomal RNA.

BP 14.80 Tue 18:00 P2

**Multiplexed magnetic tweezers for high-throughput measurements** — •LEONHARD SCHATT, STEFANIE D. PRITZL, ALPTUĞ ULUGÖL, and JAN LIPPERT — University of Augsburg, Augsburg, Germany

Single-molecule techniques, such as magnetic tweezers, are powerful tools for studying forces and torques on the nanoscale. However, throughput in single-molecule measurements can still be limiting. To solve this problem, we present a multiplexed magnetic tweezer setup that can perform real-time high-throughput force and torque measurements. In addition, our setup enables controlled excitation in the UV and visible range, to study the response to photo-triggers and photo-excitation.

BP 14.81 Tue 18:00 P2

**Pulling Geometry as a Design Parameter for Coiled Coil-Based Molecular Force Sensors** — •LAURA M. WOLFHÄLER<sup>1</sup>, ZEYNEP ATRIS<sup>2</sup>, ANGELO VALLERIANI<sup>2</sup>, RUSSELL J. WILSON<sup>1,2</sup>, and KERSTIN G. BLANK<sup>1,2</sup> — <sup>1</sup>Johannes Kepler Universität, Linz, Austria — <sup>2</sup>Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Molecular force sensors (MFSs) measure piconewton-scale forces central to cell adhesion, migration and differentiation. While DNA-based MFSs are well established, their functionalization requires multistep chemistry. We introduce a protein-based MFS building block derived from heterodimeric coiled coils (CCs). Building on our prior work showing how CC length, helix stability and core packing shape mechanics, we now identify pulling geometry as a powerful and versatile parameter for tuning CC mechanical stability without altering thermodynamic or kinetic properties. Using atomic force microscope-based single-molecule force spectroscopy, we applied force parallel and perpendicular to the CC superhelix and observed strongly geometry-dependent rupture forces, including distinct responses for the two shear modes of a 4-heptad heterodimer. These results highlight how local helix stability and structural anisotropy determine CC mechanical behavior. This work establishes a foundation for using MFSs across a wide range of cell culture applications. Their ability to report forces at molecular scales could transform how mechanical signaling is studied at cell-material interfaces.

BP 14.82 Tue 18:00 P2

**Thermal noise particle tracking and interaction measurements at interfaces under minimal external force** — •NILS LE COUTRE and ALEXANDER ROHRBACH — Bio- and Nano-Photonics, IMTEK, University of Freiburg, Germany

Forces play a vital role in experimental biophysics. From receptor-binding studies to flow-drag analysis, understanding the magnitude, direction, and origin of these forces is essential for uncovering underlying mechanisms. Optical tweezers are widely used in this context because they not only enable the measurement of biophysical interactions, but also deliberately manipulate a biological system to trigger and observe otherwise highly unlikely yet relevant interactions between the system's individuals.

To leverage this advantage for studying specific interaction processes, a robust understanding of the probe position distributions, defined by both the trapping and the surface potential and the interferometric tracking response is required, especially near interfaces and surfaces such as cell membranes. We discuss the question how far an optical trap has to approach an interface such that a natural interaction process between two binding partners is enabled (e.g. receptor on surface and ligand in optical trap).

In this presentation, I expound experiments by exploring the underlying theory and by conducting benchmark measurements in electrolyte-controlled systems, characterizing the behavior of trapped probes as their microscopic environment is altered.

BP 14.83 Tue 18:00 P2

**Plasma elastic properties in cross microchannels** — •MICHELLE

KRON, JOSÉPHINE VAN HULLE, and CHRISTIAN WAGNER — Experimental Physics Saarland University

Cross-slot microfluidic geometries produce planar extensional flows and are used to investigate flow instabilities in Newtonian and complex fluids. In Newtonian liquids, an inertial instability produces a steady vortex beyond a critical Reynolds number. In viscoelastic polymer solutions, elastic stresses near the stagnation point lower this threshold. Here we investigate human plasma, which is weakly elastic under extensional flow. Using cross-slot experiments, we quantify how plasma elasticity shifts the Reynolds number threshold for vortex onset and compare the impact of common anticoagulants on this response. We show that plasma reduces the Reynolds-number threshold for vortex onset, underscoring the importance of considering its weak elasticity for physiological studies.

BP 14.84 Tue 18:00 P2

**Effective binary models of multicomponent phase separation** — •HENRI SCHMIDT and DAVID ZWICKER — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Biological cells rely on biomolecular condensates for spatiotemporal organization. Condensates consist of many differently interacting biomolecules, which leads to a rich and complex configuration space.

Yet, only a few types of molecules can be measured in experiments, and the resulting phase behavior is typically explained using low-dimensional models. To understand the conditions under which such dimensionality reduction is feasible, we numerically explore multicomponent phase separation and ask when the behavior of a particular component can be explained by simple binary phase separation. This is surprisingly often the case, even when the unobserved components undergo phase separation on their own. However, the predicted interaction parameters and molecular volumes typically deviate from their true values, indicating that the reduction introduced systematic measurement errors.

Understanding the details of the dimensionality reduction will allow us to better probe multicomponent phase separation by observing a few components in the future.

BP 14.85 Tue 18:00 P2

**Dynamics of tissue sampling of resident tissue macrophages** — •MIRIAM SCHNITZERLEIN<sup>1,2</sup>, ERIC GRETO<sup>3,4</sup>, STEFAN UDERHARDT<sup>3,4</sup>, and VASILY ZABURDAEV<sup>1,2</sup> — <sup>1</sup>Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen — <sup>2</sup>Max-Planck-Zentrum für Physik und Medizin, Erlangen — <sup>3</sup>FAU und Universitätsklinikum Erlangen — <sup>4</sup>Optical Imaging Competence Center Erlangen, FAU

Resident tissue macrophages (RTMs) are a type of immune cell present in essentially every tissue in the human body. One of their main functions is to keep the tissue in homeostasis by resolving lesions or removing dead cells, thereby preventing unnecessary inflammation and avoiding collateral damage to the tissue. To find such incidents, RTMs show continuous sampling behaviour by extending and retracting cell protrusions. This sampling behaviour needs to be tightly regulated - due to finite amounts of available cell cytoplasm and membrane - while still guarding the entirety of the tissue.

In this project, we have employed a high-resolution, intravital imaging protocol to generate dynamic data of murine RTMs *in vivo* in the peritoneum. Next we have built a custom image processing pipeline to segment RTM protrusions and their dynamic behaviour. We could then analyse the sampling range of protrusions and found correlations between outgrowth and shrinking of protrusions. Furthermore, the data hints at a division of labour approach protrusions employ when scanning the tissue.

BP 14.86 Tue 18:00 P2

**Bottom-up emergence of a primitive replicator** — •MAGDALENA HÄUPL, IVAR HAUGERUD, and CHRISTOPH WEBER — Faculty of Mathematics, Natural Sciences, and Materials Engineering: Institute of Physics, University of Augsburg, Universitätsstraße 1, 86159 Augsburg, Germany

Non-equilibrium selection pressures were proposed as a mechanism of forming oligonucleotides whose sequences encode rich functionalities, including 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 develop a non-equilibrium thermodynamic theory to describe oligomerization, templated ligation, and se-

quence fragmentation away from equilibrium and under non-dilute conditions prone to phase separation.

We show the emergence of a strong selection mechanism. Most strikingly, a primitive replicator arises that is solely based on the inter-sequence interactions that drive sequence condensation. These results highlight that out-of-equilibrium condensed phases may provide versatile hubs for Darwinian-like evolution toward functional sequences, both relevant for the molecular origin of life and *de novo* life.

BP 14.87 Tue 18:00 P2

**Wetting of Chemically Active Condensates on Membranes** — •MENGMEI WU and DAVID ZWICKER — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

Droplets undergo partial spreading, division, merging, engulfment, and exocytosis in cellular environments. When these droplets are chemically active, as is common for many condensates in cells, the resulting long-range fluxes further enrich and modify these behaviors. To analyze the interplay between chemically active droplets and membranes, we develop a coarse-grained molecular dynamics model together with a continuum theory based on Cahn-Hilliard reaction-diffusion dynamics coupled to membrane curvature elasticity. Our approach demonstrates how chemical reactions and the resulting fluxes control both droplet morphology and membrane deformation, providing physical insight for cellular condensates as well as for the design of synthetic responsive membrane-droplet systems.

BP 14.88 Tue 18:00 P2

**staged self-organized attack mechanisms of camponotus japonicus against intruders** — •YIFAN ZHANG and ZHANGANG HAN — School of Systems Science, Beijing Normal University, Beijing, China

Social insect colonies display complex collective behaviors that emerge from local interactions, enabling decentralized strategies to counter external threats. Although ant collective activities such as foraging and nest construction are well studied, the self-organized attack mechanisms ants employ against specific intruders remain poorly understood. Using the *camponotus japonicus* and earwigs as research subjects, we show that ants exhibit a staged escalation pattern when confronting an invader: from individual probing, to small-group containment, and ultimately large-scale coordinated assaults. Building on a master-equation framework, we establish continuous-space dynamical equations and propose an ant attack behavior model to characterize these processes. Notably, the collective attack displays strong nonlinear synergy\*six ants generate an attack intensity far exceeding a simple tripling of that from two ants. These findings highlight the adaptive advantages of coordinated aggression, demonstrating how cooperative interactions among individuals greatly amplify group-level defensive efficiency. Our study offers new insights into how decentralized biological systems achieve swarm intelligence and produce emergent combat behavior, and clarifies the role of self-organization in shaping effective group decision-making.

BP 14.89 Tue 18:00 P2

**Protein self-assembly, infinitely complex yet simple?** — •LUKAS KALVODA<sup>1</sup> and MARTIN LENZ<sup>1,2</sup> — <sup>1</sup>LPTMS, CNRS, Université Paris-Saclay — <sup>2</sup>PMMH, CNRS, ESPCI Paris, PSL University

Cells rely on protein self-assembly to form functional complexes, but a lack of regulation gives rise to pathological fibers in diseases like Alzheimer's and sickle cell anemia. Why proteins robustly form these well-defined morphologies is largely unknown.

Beyond the molecular details, the complexity of proteins in shape and interactions suggests that their self-assembly may be governed by the laws of statistical physics. We introduce an analytical lattice model of anisotropic self-assembling particles to study what we term the “infinite complexity limit”. Therein the number of distinct interactions grows to infinity. Strikingly, in this limit, the “molecular” details of the interactions do not matter anymore. Instead their distribution and extreme value statistics determine the self-assembly outcome.

BP 14.90 Tue 18:00 P2

**From Individuals to Waves: Mechanisms Shaping Collective Responses in Sulphur Mollies** — •BIANCA PACINI<sup>1</sup>, YUNUS SEVINCHAN<sup>1,3</sup>, DAVID BIERBACH<sup>2,3</sup>, KORBINIAN PACHER<sup>2,3</sup>, JENS KRAUSE<sup>2,3</sup>, and PAWEŁ ROMANCZUK<sup>1,3</sup> — <sup>1</sup>Institute for Theoretical Biology, HU Berlin, Berlin, Germany — <sup>2</sup>Leibniz-Institute of Freshwater Ecology and Inland Fisheries, Berlin, Germany — <sup>3</sup>Science of

Intelligence, TU Berlin, Berlin, Germany

Collective biological systems, from neuronal networks to animal groups, exhibit the remarkable ability to rapidly modify their collective behaviour in response to changing environmental cues. By integrating local interactions with external information, they achieve flexible and coordinated group-level responses.

We investigated large fish shoals of sulphur mollies (*Poecilia sulphuraria*) in Southern Mexico, which perform collective diving cascades as a response to predation, producing wave-like patterns on the water surface. Interestingly, as a form of collective perception, we found that the group responds as a unified entity, showing a gradual stimulus-response pattern in their initial reaction.

Informed by empirical patterns extracted from a large video dataset of surface waves triggered by synthetic stimuli or bird attacks, we developed an agent-based model which captures the system's essential features. Systematic exploration of the model identifies the key individual-level mechanisms driving collective dynamics and shows how changes in local behaviour can drive collective adaptations across ecological contexts.

BP 14.91 Tue 18:00 P2

**Confirmation of Jarzynski's equality based on single molecular and macroscopic interaction force measurements** — •IAGO PETERS, LAURA MEARS, STEFAN SZOKOLL, and MARKUS VALTNER — TU Wien, Wien, Austria

Knowledge about the free energy landscape of biomolecular reactions is necessary to understand how life works on the smallest scale. Unfortunately, obtaining experimental values of the free energy difference between two states like an unbound and a bound state of two molecules is rather difficult. Jarzynski proposed an equality that connects the free energy difference between two states with the irreversible work that leads from one state to the other. Precisely, an average of all possible realizations of a process that moves the system from an equilibrium state to another state in equilibrium. Here, we test this hypothesis with experimental values. Using a simple model system, the different nucleobase-pair interactions are measured using three different techniques that are able to measure the interaction forces between two single molecules and up to several million interactions in a single experiment run. Using the Atomic Force Microscope (AFM), Optical Tweezers and the Surface Force Apparatus allows us to additionally investigate the scaling of biological single molecule interactions. Together with molecular dynamics simulations a strong foundation is laid to confirm Jarzynski's equality and investigate the scaling of single-molecule interactions.

BP 14.92 Tue 18:00 P2

**Phase separation in chemically reacting systems controls cross-phase pH difference** — •LINGE LI, OMAR ADAME-ARANA, and FRANK JÜLICHER — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187, Dresden

Biomolecular condensates are increasingly recognized as dynamic chemical environments whose properties are strongly modulated by their pH environment. Recent experiments have focused on the pH differences between the coexisting liquid phases, but a minimal theoretical framework that can account for these observations and elucidating their physical principles is still lacking. Here, we develop a minimal thermodynamic model that integrates charge-regulated macromolecules and their counterions. By identifying the conjugate thermodynamic variables constrained by chemical equilibrium and charge neutrality, we construct the thermodynamics at equilibrium and uncover a variety of phase behaviors. We show that asymmetric partitioning of ions in phase separated compartments naturally generates electric potential and pH differences, with the dense-phase pH consistently buffered toward the macromolecular isoelectric point. We further demonstrate that these pH differences are governed by macromolecular interactions and molecular properties. Together, our results suggest that phase separation provides a robust mechanism for buffering dilute-phase pH variations and enabling controlled modulation of pH in the presence of condensates. The framework uncovers general physical principles of how pH regulation can be achieved phase-separated environments.

BP 14.93 Tue 18:00 P2

**Phase separation in chemically reacting systems controls cross-phase pH difference** — LINGE LI, •OMAR ADAME-ARANA, and FRANK JÜLICHER — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187, Dresden

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BP 14.94 Tue 18:00 P2

**Statistical mechanics of disordered buckling instabilities** — •TANGDI LUAN<sup>1,2,3</sup> and PIERRE A. HAAS<sup>1,2,3</sup> — <sup>1</sup>Max Planck Institute for the Physics of Complex Systems — <sup>2</sup>Max Planck Institute of Molecular Cell Biology and Genetics — <sup>3</sup>Center for Systems Biology Dresden

Buckling instabilities drive the emergence of biological shape during morphogenesis, but the effect of the large variability of these systems at the microscopic cell scale on these instabilities at the macroscopic scale of tissues is largely unknown. The buckling of a rod with disordered growth [1] is perhaps the simplest setup of this problem. Numerical simulations [1] reveal that even in this minimal setup, the distribution of growth disorder has complex effects on the buckling threshold.

Here, we provide the theoretical underpinnings for these observations: we develop the statistical theory that explains how the spatial distributions of disorder of growth and material properties conspire to determine the threshold for the instability. Our results thus indicate how correlations and hence feedbacks between stress and growth can control mechanical instabilities and, by extension, the emergence of biological shape in development.

[1] Ramachandran *et al.*, Phys. Rev. E **110** (2024)

BP 14.95 Tue 18:00 P2

**Exchange controls coarsening of surface condensates** — •RICCARDO ROSSETTO<sup>1,2</sup>, MARCEL ERNST<sup>1,2</sup>, GERRIT WELLECKE<sup>1,2</sup>, and DAVID ZWICKER<sup>1</sup> — <sup>1</sup>Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — <sup>2</sup>University of Göttingen, Institute for the Dynamics of Complex Systems, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Biological membranes often exhibit heterogeneous protein patterns, which cells control. Strong patterns, like the polarity spot in budding yeast, can be described as surface condensates formed by physical interactions between constituents. However, it is unclear how these interactions affect the material exchange with the bulk. To study this, we analyze a thermodynamically consistent model which reveals that passive exchange leads to new equilibrium phenomena, such as re-entrant phase transitions, and generally accelerates the coarsening of surface condensates. Active exchange can further accelerate coarsening, although it can also fully arrest it and induce complex patterns involving various length scales. We reveal how these behaviors are related to non-local transport via diffusion through the bulk, rationalizing the various scaling laws we observe and allowing us to interpret biologically relevant scenarios.

BP 14.96 Tue 18:00 P2

**Noisy mixtures at the mesoscale: Vacuoles dancing in chemically active droplets** — •ESTÉBAN ARASPÍN, LEONARDO SILVA DIAS, and CHRISTOPH A. WEBER — Faculty of Mathematics, Natural Sciences, and Materials Engineering: Institute of Physics, University of Augsburg, Universitätsstrasse 1, 86159 Augsburg, Germany

Understanding biological mixtures at the mesoscale calls for models that connect microscopic reactions with emergent continuum behavior in a thermodynamically consistent way. At such coarse-grained

scales, noise, generally of multiplicative nature, is essential to capture phenomena like nucleation or stochastic switching between non-equilibrium steady states.

We developed a theoretical framework based on effective mesoscopic reaction-diffusion master equations that is applicable to both passive systems and non-equilibrium scenarios in which chemostatted fluxes make the mixture active. The framework connects to the macroscopic limit, recovering reactive Cahn-Hilliard-Cook dynamics.

As an application, we explore chemically active droplets in which a

chemostatted ATP concentration leads to striking morphological dynamics. We find dilute-phase vacuoles that form and dissolve, reminiscent of bubbly phase separation in Model B+. We observe growth of small vacuoles at the expense of larger ones, dynamics that can be considered an inverse-ripening process.

Our results highlight the value of mesoscopic stochastic frameworks for understanding active phase separation and other soft-matter systems maintained away from equilibrium.