Biological Physics Division
Fachverband Biologische Physik (BP)

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Overview of Invited Talks and Sessions

(Lecture halls BAR Schö, TOE 317, and BAR 0106; Poster P1 and P2/EG)

Invited Talks

BP 1.7	Mon	11:15–11:45	BAR Schö	**Cell-free expression of membrane proteins and control of their spatial organization in synthetic lipid membranes** — •Jan Steinkühler
BP 2.1	Mon	9:30–10:00	TOE 317	**Emergent properties in motile active matter** — •Roland G. Winkler
BP 3.5	Mon	10:30–11:00	BAR 0106	**Resolving gating and allosteric modulation in ion channels through simulations and small-angle neutron scattering** — •Erik Lindahl
BP 5.1	Mon	15:00–15:30	TOE 317	**Repurposing nucleic acids as high-resolution force sensors: From fundamental mechanotransduction to translational biophysics** — •Khalid Salaita
BP 6.5	Mon	16:15–16:45	BAR 0106	**Mechanical and electrical properties of bacterial biofilms modulate antibiotic tolerance** — •Berenike Maier
BP 8.5	Tue	10:45–11:15	BAR Schö	**Microtubule Lattice Dynamics** — Subham Biswas, Rahul Grover, Cordula Reuther, Mona Grünewald, Stefan Diez, •Laura Schaedel
BP 10.1	Tue	9:30–10:00	BAR 0106	**Protein evolution in sequence landscapes: from data to models and back** — •Martin Weigt
BP 12.4	Wed	10:15–10:45	TOE 317	**Materials properties of bacterial biofilms.** — •Cécile M. Bidan
BP 13.1	Wed	9:30–10:00	BAR 0106	**Biological signal processes across scales** — •Steffen Rulands
BP 16.1	Wed	11:15–11:45	BAR 0106	**Systems biophysics of bacterial response to cell wall-targeting antibiotics** — Rebecca Brouwers, Sharareh Tavaddod, Leonardo Mancini, Jacob Biboy, Elizabeth Tatham, Pietro Cicuta, Waldemar Vollmer, •Rosalind Allen
BP 21.7	Thu	11:15–11:45	BAR Schö	**Visualizing the inner life of microbes** — •Ulrike Endesfelder
BP 22.5	Thu	10:30–11:00	TOE 317	**Statistical Physics of Spatially Organized Catalytic Particles** — •Ulrich Gerland
BP 23.1	Thu	9:30–10:00	BAR 0106	**Conformational dynamics of SARS-CoV-2 spike protein modulates the binding affinity to ACE2** — Fidan Sumbul, Claire Valotteau, Prithwidip Saha, Ignacio Fernadez, Annalisa Meola, Eduard Baquero, Dorota Kostrz, James R Portman, François Stransky, Pablo Guardado Calvo, Charlie Gosse, Terence Strick, Felix Rey, •Felix Rico
BP 26.1	Thu	15:00–15:30	TOE 317	**Decoding Molecular Plasticity in the Dark Proteome of the Nuclear Transport Machinery** — •Edward Lemke
BP 30.1	Fri	9:30–10:00	TOE 317	**Experiments on Active Polymer-Like Worms** — •Antoine Deblais, Daniel Bonn, Sander Woutersen
BP 32.1	Fri	12:15–13:00	HSZ 03	**The physical regulation of brain development** — •Kristian Franze

Invited Talks of the joint Symposium Dynamics of Opinion Formation – From Quorum Sensing to Polarization (SYOF)

See SYOF for the full program of the symposium.

SYOF 1.1	Mon	9:30–10:00	HSZ 01	**Towards understanding of the social hysteresis – insights from statistical physics** — •Katarzyna Sznajd-Weron
SYOF 1.2	Mon	10:00–10:30	HSZ 01	**Polarization in attitude distributions from surveys and models of continuous opinion dynamics** — •Jan Lorenz, Martin Gestefeld
SYOF 1.3	Mon	10:30–11:00	HSZ 01	**Collective patterns and stable misunderstandings in networks striving for consensus without a common value system** — •Johannes Falk, Edwin Eichler, Katja Windt, Marc-Thorsten Hütt
SYOF 1.4	Mon	11:15–11:45	HSZ 01	**A yet undetected cognitive bias, revealed by opinion dynamics simulations** — •Guillaume Deffuant
SYOF 1.5	Mon	11:45–12:15	HSZ 01	**Extreme switches in kinetic exchange models of opinion.** — •Parongama Sen, Kathakali Biswas

Invited Talks of the joint Symposium SKM Dissertation Prize 2023 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ 04	**Diffusion of antibodies in solution: from individual proteins to phase separation domains** — •Anita Girelli
SYSD 1.2	Mon	10:00–10:30	HSZ 04	**Intermediate Filament Mechanics Across Scales** — •Anna V. Schepers
SYSD 1.3	Mon	10:30–11:00	HSZ 04	**Ultrafast Probing and Coherent Vibrational Control of a Surface Structural Phase Transition** — •Jan Gerrit Horstmann
SYSD 1.4	Mon	11:00–11:30	HSZ 04	**Electro-active metasurfaces employing metal-to-insulator phase transitions** — •Julian Karst
SYSD 1.5	Mon	11:30–12:00	HSZ 04	**The role of unconventional symmetries in the dynamics of many-body systems** — •Pablo Sala

Invited Talks of the joint Symposium Physics of Fluctuating Paths (SYFP)

See SYFP for the full program of the symposium.

SYFP 1.1	Tue	9:30–10:00	HSZ 01	**Time at which a stochastic process achieves its maximum** — •Satya Majumdar
SYFP 1.2	Tue	10:00–10:30	HSZ 01	**Fluctuations and molecule-spanning dynamics of single Hsp90 proteins on timescales from nanoseconds to days** — •Thorsten Hugel
SYFP 1.3	Tue	10:30–11:00	HSZ 01	**Path reweighting for Langevin dynamics** — •Bettina Keller
SYFP 1.4	Tue	11:15–11:45	HSZ 01	**Out-of-equilibrium dynamics of trapped Brownian particles** — •Raul A. Rica
SYFP 1.5	Tue	11:45–12:15	HSZ 01	**Thermodynamics of Clocks** — •Patrick Pietzonka

Invited Talks of the joint Symposium Topology in Quantum and Classical Physics – From Topological Insulators to Active Matter (SYQC)

See SYQC for the full program of the symposium.

SYQC 1.1	Wed	15:00–15:30	HSZ 01	**Topological magnetic whirls for computing** — •Karin Everschor-Sitte
SYQC 1.2	Wed	15:30–16:00	HSZ 01	**Topological waves from solids to geo/astrophysical flows** — •Pierre Delplace, Antoine Venaille, Nicolas Perez, Guillaume Laibe, Armand Leclerc, Manolis Perrot, Brad Marston
SYQC 1.3	Wed	16:00–16:30	HSZ 01	**Topological Phase Transitions in Population Dynamics** — •Erwin Frey
SYQC 1.4	Wed	16:45–17:15	HSZ 01	**Topological invariants protect robust chiral currents in active matter** — •Evelyn Tang
SYQC 1.5	Wed	17:15–17:45	HSZ 01	**Topological defects in biological active matter** — •Amin Doostmohammadi

Sessions

BP 1.1–1.12	Mon	9:30–13:00	BAR Schö	**Membranes, Vesicles, Synthetic Cells**
BP 2.1–2.12	Mon	9:30–13:00	TOE 317	**Active Matter I (joint session BP/CPP/DY)**
BP 3.1–3.12	Mon	9:30–13:00	BAR 0106	**Computational Biophysics I**
BP 4.1–4.9	Mon	15:00–17:30	BAR Schö	**Tissue Mechanics I**
BP 5.1–5.8	Mon	15:00–17:30	TOE 317	**Focus Session NanoAgents**
BP 6.1–6.7	Mon	15:00–17:15	BAR 0106	**Bacterial Mechanics**
BP 7.1–7.11	Mon	15:00–18:15	ZEU 160	**Active Matter II (joint session DY/BP/CPP)**
BP 8.1–8.11	Tue	9:30–13:00	BAR Schö	**Cell Mechanics I**
BP 9.1–9.11	Tue	9:30–12:30	TOE 317	**Active Matter III (joint session BP/CPP/DY)**
BP 10.1–10.9	Tue	9:30–12:15	BAR 0106	**Evolution and Origin of Life**
BP 11.1–11.78	Tue	12:30–15:30	P1	**Poster Session I**
BP 12.1–12.12	Wed	9:30–13:00	TOE 317	**Biopolymers and Biomaterials (joint session BP/CPP)**
BP 13.1–13.5	Wed	9:30–11:00	BAR 0106	**Signaling, Biological Networks**
BP 14.1–14.10	Wed	9:30–13:00	ZEU 160	**Focus Session: From Inter-individual Variability to Heterogeneous Group Dynamics and Disorder in Active Matter (joint session DY/BP/CPP)**
BP 15.1–15.6	Wed	10:30–12:15	BAR Schö	**Tissue Mechanics II**
BP 16.1–16.6	Wed	11:15–13:00	BAR 0106	**Systems Biophysics**
BP 17.1–17.9	Wed	15:00–17:30	BAR 0106	**Protein Structure and Dynamics**
BP 18.1–18.6	Wed	15:00–16:30	ZEU 250	**Biologically Inspired Statistical Physics (joint session DY/BP)**
BP 19.1–19.6	Wed	16:30–18:00	MER 02	**Biopolymers, Biomaterials and Bioinspired Functional Materials (joint session CPP/BP)**
BP 20	Wed	18:00–19:00	BAR Schö	**Members' Assembly**
BP 21.1–21.12	Thu	9:30–13:00	BAR Schö	**Bioimaging**
BP 22.1–22.12	Thu	9:30–13:00	TOE 317	**Statistical Physics of Biological Systems I (joint session BP/DY)**
BP 23.1–23.12	Thu	9:30–13:00	BAR 0106	**Single Molecule Biophysics**
BP 24.1–24.12	Thu	9:30–13:00	ZEU 160	**Active Matter IV (joint session DY/BP/CPP)**
BP 25.1–25.9	Thu	15:00–17:30	BAR Schö	**Cell Mechanics II**
BP 26.1–26.8	Thu	15:00–17:30	TOE 317	**Focus Session mRNA Physics**
BP 27.1–27.9	Thu	15:00–17:30	BAR 0106	**Computational Biophysics II**
BP 28.1–28.58	Thu	18:00–20:00	P2/EG	**Poster Session II**
BP 29.1–29.9	Fri	9:30–12:00	BAR Schö	**Statistical Physics of Biological Systems II (joint session BP/DY)**
BP 30.1–30.8	Fri	9:30–12:00	TOE 317	**Active Matter V (joint session BP/CPP/DY)**
BP 31.1–31.7	Fri	10:00–12:00	BAR 0106	**Cell Mechanics III**
BP 32.1–32.1	Fri	12:15–13:00	HSZ 03	**Closing Plenary Talk (joint session BP/CPP)**

Members' Assembly of the Biological Physics Division

Wed 18:00–19:00 BAR Schö

BP 1: Membranes, Vesicles, Synthetic Cells

Time: Monday 9:30–13:00 Location: BAR Schö

BP 1.1 Mon 9:30 BAR Schö

Bottom-up assembly of a synthetic glycocalyx on lipid vesicles — •Kevin Jahnke and David A. Weitz — Harvard University, Cambridge, MA, USA

The glycocalyx serves as physicochemical barrier that increases cellular rigidity and as interface for chemical cues to guide cell-cell communication. However, while preliminary results highlight the importance of the glycocalyx, the biophysical functioning remained elusive and mostly untested due to the complexity within natural cells. Recent advances in the membrane functionalization of giant unilamellar vesicles (GUVs) with macromolecules like DNA and proteins (Jahnke et al., ACS Nano 2022; Jahnke et al. Nat. Commun. 2021) pave the way for a systematic investigation of glycocalyx properties within a fully-controlled environment. Here, we engineer biomimetic glycocalyces to understand their effect on the biophysical properties of GUVs. The synthetic glycocalyx consists of polysaccharides functionalized with cholesterol that self-assemble in the lipid membrane. We employ fluorescence recovery after photobleaching and micropipette aspiration to assess the changes in diffusion and membrane rigidity of glycocalyx-decorated GUVs. The control over the type of polysaccharide, its molecular weight and density on the vesicle enable us to design and study a variety of synthetic glycocalyces. Additionally, we compare them to other common vesicle functionalizations like polyethyleneglycol and explore their potential for carbohydrate-specific adhesion. This work underpins bottom-up glycocalyx engineering as important tool for cellular biophysics and biotechnological applications.

BP 1.2 Mon 9:45 BAR Schö

Surface-induced phase separation of reconstituted nascent integrin clusters — •Chiao-Peng Hsu[1], Jonas Aretz[2], Reinhard Fässler[2], and Andreas Bausch[1] — [1]Center for Functional Protein Assemblies and Lehrstuhl für Zellbiophysik (E27), Physics Department, Technische Universität München, Garching, Germany — [2]Max Planck Institute of Biochemistry, Martinsried, Germany

Integrin adhesion complexes are essential membrane-associated cellular compartments for multi-cellular life. While biomolecular condensates organize specific functions in cells, cell membranes can regulate the positions and dynamics of many biomolecular condensates. Yet, the role played by membrane surfaces in the formation of initial integrin adhesion complexes still needs to be fully understood. Here, we report that phosphoinositides containing lipid membranes induce minimal integrin adhesion condensates composed of integrin β tails, kindlin, talin, paxillin, and FAK at physiological ionic strengths and protein concentrations. We show that the presence of phosphoinositides is key to enriching kindlin and talin on the membrane, forming first nascent integrin complexes, which in turn are necessary to further nucleate condensates. These results demonstrate that the biophysical properties of lipid membranes are key for inducing specific membrane-associated condensates throughout the cell.

BP 1.3 Mon 10:00 BAR Schö

Small-Angle and Inelastic Neutron Scattering from Polydisperse Oligolamellar Vesicles Containing Glycolipids — •Lukas Bange[1], Ingo Hoffmann[2], and Emanuel Schneck[1] — [1]Institute for Condensed Matter Physics, Technical University Darmstadt, Germany — [2]nstitut Laue-Langevin, Grenoble, France

Glycolipids are known to stabilize biomembrane multilayers through preferential sugar-sugar interactions that act as weak transient membrane crosslinkers [1, 2]. We use small-angle and inelastic neutron scattering on oligolamellar phospholipid vesicles containing defined glycolipid fractions in order to elucidate the influence of glycolipids on membrane mechanics and dynamics. Small-angle neutron scattering (SANS) reveals that the oligolamellar vesicles (OLVs) obtained by extrusion are polydisperse with regard to the number of lamellae, n, which renders the interpretation of the inelastic neutron spin echo (NSE) data [3] non-trivial. To overcome this problem, we propose a method to model the NSE data in a rigorous fashion based on the obtained histograms of n and on their q-dependent intensity-weighted contribution. This procedure yields meaningful values for the bending rigidity of individual lipid membranes and insights into the mechanical coupling between adjacent membrane lamellae, including the effect of the glycolipids.

References [1] Latza, Demé, Schneck, Biophys J., 2020, Volume 118, 7, P1602-1611 [2] Kav et al, Front. Mol. Biosci., 2021, 8, 754645 [3] Hoffmann, Hoffmann, Farago, Prevost, Gradzielski, J. Chem. Phys., 2018, 148, 104901

BP 1.4 Mon 10:15 BAR Schö

Controlling phase separations and reaction kinetics in microfluidically trapped droplets — •Sebastian W. Krauss, Paula Girones Paya, and Matthias Weiss — Experimental Physics I, University of Bayreuth, Germany

Droplet-based microfluidics is an efficient and versatile tool to study biomimetic reactions and self-organization in selected geometries and small volumes. It is also frequently used to perform high-throughput experiments, e.g. as selection platforms for directed evolution or for personalised medicine. While elaborate techniques are available for the production of picoliter-sized droplets, there is an increasing demand for subsequent manipulation and control of the droplet interior after production. Here we report on a straightforward method to rapidly and reversibly adjust the size of single to several hundred double-emulsion droplets in a microfluidic sieve by varying the osmotic pressure, leading to a change in concentration of enclosed molecules. We show that this approach allows for driving reversible demixing transitions of a biomimetic binary fluid which can be used to control the kinetics of enclosed enzymatic reactions. We also show that changing droplet sizes can be exploited for a reversible denaturing of double-stranded DNA, which may eventually allow for an osmotically driven PCR in small droplets.

BP 1.5 Mon 10:30 BAR Schö

Predicting membrane turnover during cytokinesis — •Felix Frey[1] and Timon Idema[2] — [1]Institute of Science and Technology Austria, Klosterneuburg, Austria — [2]Department of Bionanoscience, Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands

When animal cells divide, they split into two equal parts. Since the volume of the cell is typically conserved during cell division, the projected area of the cell membrane has to increase to allow for the change of shape. The membrane area is controlled by exocytosis, resulting in an increase in membrane area and its counterpart endocytosis, resulting in a decrease in membrane area. However, it is unclear how exo- and endocytosis need to adapt to enable successful division. To address this question, we developed a kinetic model in which membrane gain and loss depend on membrane curvature and tension [1]. We apply this model to a series of calculated vesicle shapes, which we take as a proxy for the shape of dividing cells. We find that the ratio of membrane gain and loss changes non-monotonically during cytokinesis due to the complex interplay between membrane area and shape. Our results suggest that controlling membrane turnover is critical for the successful division of both biological and artificial cells. [1] Felix Frey and Timon Idema, Phys. Rev. E 106, 024401 (2022).

BP 1.6 Mon 10:45 BAR Schö

Antimicrobial peptides: Revealing the Penetration Mechanism of Melittin in the Outer Membrane of Gram-Negative Bacteria — •Justus C. Stephani[1], Luca Gerhards[1], Ilia A. Solov'yov[1], and Izabella Brand[2] — [1]Dept. of Physics, Carl von Ossietzky Universität, Germany — [2]Dept. of Chemistry, Carl von Ossietzky Universität Oldenburg, Germany

Studying the interaction between antimicrobial peptides (AMPs) and bacterial membranes might aid to find new treatments against bacterial pathogens and even drug-resistant bacteria. The AMP melittin can target the complex structure of a cell membrane leading to membrane permeabilization via hole formation or disruption. We report on the results of electrochemical experiments, aided by modern, all-atom molecular dynamics simulations that reveal the role of lipopolysaccharides (LPS) in the outer membrane of gram-negative bacteria in melittin binding and penetration. We demonstrate that certain amino acid residues play a key role in the binding of melittin to the membrane and thereby stabilizing and preserving the confirmation of the peptide. With a combined method of polarization modulation infrared reflection-absorption spectroscopy (PM IRRAS) and the statistical analysis of C=O bond orientation in the peptide, we determine

the orientation of melittin on the membrane and observed penetration of the N-Terminus of the peptide into the membrane and a formation of hydrogen bonds between the N-Terminus and carboxylate and phosphate of the LPS.

15 min. break

Invited Talk BP 1.7 Mon 11:15 BAR Schö

Cell-free expression of membrane proteins and control of their spatial organization in synthetic lipid membranes — •Jan Steinkühler — Northwestern University, Evanston, USA — Georg-August-Universität Göttingen, Germany

Cell-free expression (CFE) is a powerful tool for synthesizing proteins outside of living cells, including membrane proteins. In this talk, we will discuss the factors that affect the yield of synthesized membrane proteins in CFE systems, including ribosome stalling and the balance between peptide-membrane association and peptide aggregation rates. We will also present a quantitative kinetic model that can be used to rationalize the engineering of protein N-terminal domain sequences and membrane composition for improved membrane protein synthesis. In addition to covering the synthesis of natural membrane proteins, we will show how CFE of de novo membrane protein designs can be used to study the role of membrane-protein hydrophobic mismatch in protein integration and organization in synthetic lipid membranes. [DOI:10.1101/2022.06.01.494374]. Our findings provide insight into protein organization in biological membranes and a framework for building up of synthetic cell membranes with new functions.

BP 1.8 Mon 11:45 BAR Schö

Entry of Microparticles into Giant Lipid Vesicles Induced by Optical Force — •Fessler Florent, Sharma Vaibhav, Muller Pierre, Thalmann Fabrice, Marques Carlos, and Stocco Antonio — Institut Charles Sadron, Strasbourg, France

Interactions between micro- or nano-sized objects and lipid membranes are crucial in many processes such as entry of viruses in host cells, microplastics pollution, drug delivery or biomedical imaging. Here, we investigated the physical principles of particle crossing of lipid membranes using microparticles and giant unilamellar vesicles (GUVs) in the absence of strong irreversible binding and for low membrane tensions. In these conditions, we observed that organic as well as inorganic particles can always penetrate inside GUVs provided that an external picoNewton force is applied. In the limit of a vanishing particle-membrane affinity, we pointed out the role of membrane area reservoirs and showed that a force barrier minimum exists when the particle size is comparable to the bendocapillary length.

BP 1.9 Mon 12:00 BAR Schö

Simulating transient pores in hemifused membranes — •Russell Spencer and Marcus Müller — Georg-August Universität Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany

Transportation of material from one side of a hemifused membrane to another can be facilitated through the formation of transient pores, which open, allow the material to pass and then close. One important example of this occurs in the 'kiss and run' (KAR) mechanism for transporting material from inside a vesicle in a cell to outside of the cell. The vesicle first fuses with the membrane, forming a hemifusion diaphragm (HD). A pore then opens in the HD allowing the material out, then the pore closes and the vesicle detaches. This process occurs in the release of neurotransmitters from a synapse into the post-synaptic cleft. This work uses self-consistent field theory and the string method to calculate the minimum free energy path for membrane fusion and the opening and closing of the transient pore. We also study the effects of proteins, which facilitate the process by altering the thermodynamics of pore formation.

BP 1.10 Mon 12:15 BAR Schö

Lipid movement in monolayers at the air/water interface: hydrodynamic coupling to the subphase — Florian Gellert, Heiko Ahrens, and •Christiane A. Helm — Institute of Physics, University of Greifswald, Germany

Domain nucleation and growth in the liquid expanded/liquid condensed (LE/LC) phase transition in erucic acid monolayers at the air/water interface is studied. Dendritic domains are observed at high compression speeds and seaweed domains at low compression speeds. The different domain types are distinguished by fractal dimension, tip width, and the spacing of the side arms. A local, normalized supersaturation describes the hydrodynamic coupling of lipids in the LE phase moving towards the domain border to subphase movement. The coupling differs for the growth regimes. Additionally, the shape and symmetry of the domains are affected by barrier movement. The downstream side of the domains grows faster than the upstream side, as shown by directionality diagrams and FFTs. We suggest that the flow direction disturbs the diffusion direction of the lipids within the LE phase but not the coupling to the subphase.

BP 1.11 Mon 12:30 BAR Schö

X-ray studies of bidirectional switching in phospholipid membranes containing photoswitchable glycolipids — •Svenja C. Hövelmann[1,2,3], Jonas E. Warias[1], Rajendra P. Giri[1], Jule Kuhn[1], Karin Hansen[1], Lukas Petersdorf[1], Nicolas Hayen[1], Philipp Jordt[1], Andrea Sartori[1], Chen Shen[3], Franziska Reise[4], Olaf M. Magnussen[1], Thisbe K. Lindhorst[4], and Bridget M. Murphy[1,3] — [1]Institute of Experimental and Applied Physics, Kiel, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [3]Ruprecht Haensel Laboratory, Kiel, Germany — [4]Otto Diels Institute of Organic Chemistry, Kiel, Germany

Lipid molecules not only play an essential role in the structure and geometry in biomembranes but also in the functionality and self-assembly of membrane proteins and channels. Their dynamic is under intense investigation owing to their applications in biosensor engineering and drug delivery. To understand the interaction between lipid and functional molecules, we investigate photoswitchable glycoconjugates embedded in a 1,2-dipalmitoyl-phosphatidylcholine (DPPC) model systems in the form of Langmuir films and vesicles. The glycoconjugates change reversibly between their trans- and cis-conformation by illumination with visible and UV light inducing a reversible change in the surrounding molecular arrangement. These structural changes, their evolution and time scales are characterised with multiple measurement techniques including X-ray scattering. Studies performed on mixed monolayers and vesicles with varying glycoconjugates identify bidirectional switching in the in DPPC monolayers.

BP 1.12 Mon 12:45 BAR Schö

Structure/Friction relationship in solid supported phospholipid layers — •Swen Helstroffer, Pierre Muller, and Thierry Charitat — Institute Charles Sadron, Strasbourg, France

Stacks of phospholipid bilayers adsorbed on biological rubbing surfaces lubricate remarkably well under severe conditions. However, the energy dissipation pathway allowing ultra low friction is still unknown. To elucidate the mechanism, we propose here to study an experimental model consisting of hydrated phospholipid layers deposited at the air/solid interface. Our system presents a well-controlled geometry in which we can fine-tune the hydration level of the lipid heads. By combining neutron reflectometry and ellipsometry studies with macroscopic tribology experiments, we demonstrated a negative correlation between hydration and friction coefficient. Using the Eyring model, we obtained microscopic activation volumes characteristic of slip. Our results suggest that the hydration level is a key parameter for lubrication. We believe that the sliding plane is located in the confined water layers.

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

Time: Monday 9:30–13:00 Location: TOE 317

Invited Talk BP 2.1 Mon 9:30 TOE 317

Emergent properties in motile active matter — •Roland G. Winkler — Theoretical Physics of Living Matter (IBI-5/IAS-2), Forschungszentrum Jülich, Jülich

Motile active matter systems, ranging from assemblies of bacteria, self-organized bio-polymers such as the cytoskeleton of living cells, to schools of fish and flocks of birds, exhibit intriguing emerging structural and dynamical out-of-equilibrium properties, even with reminiscence to classical turbulence. Their spatiotemporal dynamics is controlled by the propulsion of the active agents in combination with various direct interactions. The latter are typically anisotropic and emerge from different sources, such as elongated agent shapes, intrinsic flexibility and constraints, microswimmer flow fields etc. By analytical theory and mesoscale simulations, we study the physical aspects of motile active matter, ranging from propulsion of bacteria and linear filaments to large-scale collective properties of active agents, and unravel its generic features. Studies on individual polymers reveal fundamental differences in their dynamical and conformational properties depending on their propulsion mechanism, which is illustrated for polymers either tangentially driven or composed of active Brownian particles. In the latter case, hydrodynamic interactions additionally affect the conformational properties, in contrasts to passive polymers. Moreover, hydrodynamic interactions determine the activity-induced phase behavior. For spherical microswimmers (squirmers), hydrodynamics suppresses motility-induced phase separation, but enhances collective turbulent-like large-scale flows.

BP 2.2 Mon 10:00 TOE 317

High-resolution mapping of odd fluctuations and oscillations in living chiral crystals — •Jinghui Liu[1,2], Lisa Lin[1], Yuchao Chen[1], Yu-Chen Chao[1], and Nikta Fakhri[1] — [1]Department of Physics, Massachusetts Institute of Technology — [2]Center for Systems Biology Dresden

It has been shown that active crystals formed by self-assembling clusters of swimming starfish embryos exhibit signatures of odd mechanics, such as self-sustained chiral waves. How are these observed chiral waves and oscillations are actuated and how their dynamics couple to the formation and dissolution of the living chiral crystal? Here, we report the use of vibrational mode decomposition to dissect various non-equilibrium phases of the crystal dynamics. By analyzing embryo cluster trajectories over the time course of crystal formation and dissolution, we identify the spatial modes responsible for the collective actuation of an oscillatory active crystal both in spontaneous and mechanically excited conditions. We also report a direct extraction of dispersion relation from fluctuations of confined crystals to infer odd elastic moduli. Taken together, our results unveil the complex spatiotemporal origin of mechanical waves in non-reciprocal materials and provide insight on the design principles of collective phases of active metamaterials.

BP 2.3 Mon 10:15 TOE 317

Self-organized chemotaxis of coupled cell populations — •Mehmet Can Ucar and Edouard Hannezo — Institute of Science and Technology Austria, Am Campus 1, 3400 Klosterneuburg, Austria

Many processes in development and disease such as tissue morphogenesis, cancer invasion and immune response rely on collective directional movement of cells. In a wide array of systems this collective motility is driven locally by self-generated chemokine or stiffness gradients, as opposed to pre-patterned, global guidance cues. While recent studies have explored migration mechanisms of a single species of cells, the role of self-generated gradients navigating multiple cell types remains largely untested. Here we address this issue by introducing a theoretical framework for self-organized guidance of chemotactically coupled cell populations. Combining analytical theory and simulations with experiments on immune cell populations, we discover a diverse spectrum of collective migration patterns controlled by single-cell properties. We find that differential chemotactic sensitivity leads to efficient colocalization of distinct cell types, and show that this coupling also depends on the geometry and initial configuration of the dynamical system. We finally outline conditions for robust, sustained multicellular interactions relevant for physiological settings such as during immune response.

BP 2.4 Mon 10:30 TOE 317

Geometry-induced patterns in collective cell migration — •David Brückner — Institute of Science and Technology, Am Campus 1, 3400 Klosterneuburg, Austria

The coordinated migration of cell collectives is increasingly well understood at the level of large two-dimensional confluent monolayers. However, many physiological migration processes rely on small polarized cell clusters and their responses to external confining geometries, such as 2D channels and 3D curved environments. How active motion and cell-cell interactions interplay with such external boundaries remains poorly understood. I will discuss how external geometries can induce patterns in collective cell migration, using two examples. First, we show that the migration efficiency of 2D confined cell clusters is determined by the contact geometry of cell-cell contacts that are either parallel or perpendicular to the direction of migration. Our minimal active matter model reveals how cell-cell interactions determine a geometry-dependent supracellular stress field that controls this response to external boundaries. Secondly, we show how the interplay of curvature and active flocking dynamics of 3D cell spheroids induces a collective mode of cell migration manifesting as a propagating velocity wave. Together, these approaches provide a conceptual framework to understand how cell-cell interactions interplay with 2D and 3D geometries to determine the emergent dynamics of collective cell migration.

BP 2.5 Mon 10:45 TOE 317

Shape primed AC-electrophoretic microrobots — •Florian Katzmeier and Friedrich C. Simmel — Technical University of Munich, Munich, Germany

Second-order electrokinetic flow around colloidal particles caused by concentration polarization electro-osmosis can be utilized to controllably move asymmetric particle dimers in AC electrical fields. To demonstrate this actuation mechanism, we created particle dimers from micron-sized silica spheres with sizes 1.01 μm and 2.12 μm by connecting them with DNA linker molecules. The dimers can be steered along arbitrarily chosen paths within a 2D plane by controlling the direction of the AC electric field in a fluidic chamber with the joystick of a gamepad. Further utilizing induced dipole-dipole interactions, we demonstrate that particle dimers can be used to controllably pick up monomeric particles and release them at any desired position, and also to assemble several particles into groups. Systematic experiments exploring the dependence of the movement direction and velocity on buffer composition, frequency, and field strength further elucidate the underlying physical mechanism, and provide operational parameter ranges for our micro robotic swimmers which we termed 'SPACE-bots'.

15 min. break

BP 2.6 Mon 11:15 TOE 317

Rodrolls: self-rolling rods powered by light and chemical gradients — •Ann Rosna George[1], Martin Wittmann[2], Antonio Stocco[1], Igor M. Kulić[1], and Juliane Simmchen[2] — [1]CNRS, Institute Charles Sadron, Strasbourg, France — [2]Physical chemistry, TU Dresden, Germany

The self-rolling motion upon spontaneous symmetry breaking is demonstrated by certain rod-shaped microorganisms like viruses. Hence it is imperative that we understand the mechanism of this symmetry breaking triggering the active rolling motion. This behaviour has also been demonstrated on the macroscopic scale by rod-like objects. It is very interesting to try and replicate this on a microscopic scale. The main aim of the project is to create a new class of active rods that exhibit rolling activity under chemical and optical gradients. To achieve this, it is important to understand the mechanism of activity of rod-like objects under chemical and optical stimuli.

Experiments conducted using silica Janus rods with a Platinum layer in an aqueous solution of H2O2 give interesting results and exhibit different kinds of activity when parameters like concentration of H2O2 and aspect ratio of rods are changed. Under specific conditions, particles are capable of switching their direction of motion. Experiments

done using rods covered in gold nanoparticles under an optical gradient also reveal promising results of being able to make the rods roll upon providing sufficient energy to break the symmetry and fine-tuning certain parameters.

BP 2.7 Mon 11:30 TOE 317

Active Nematic Multipoles: Flow Responses and the Dynamics of Defects and Colloids — •Alexander J. H. Houston[1,2] and Gareth P. Alexander[1,3] — [1]Department of Physics, Gibbet Hill Road, University of Warwick, Coventry, CV4 7AL, United Kingdom — [2]Department of Physics, University of York, Heslington, York YO10 5DD, United Kingdom — [3]Centre for Complexity Science, Zeeman Building, University of Warwick, Coventry, CV4 7AL, United Kingdom

Two fundamental questions in active nematics are how to extract useful work from their non-equilibrium dynamics and how to extend the topological defect-based description of dynamics that has proved useful in two dimensions to three dimensions, in which the defects form geometrically-complex loops. We introduce a general description of localised distortions in active nematics using the framework of 'active nematic multipoles'. We give the Stokesian flows for arbitrary multipoles in terms of differentiation of a fundamental flow response and describe them explicitly up to quadrupole order. This allows the identification of the dipolar and quadrupolar distortions that generate self-propulsion and self-rotation respectively and serves as a guide for the design of arbitrary flow responses. Our results can be applied to both defect loops in three-dimensional active nematics and to systems with colloidal inclusions. They reveal the geometry-dependence of the self-dynamics of defect loops and provide insights into how colloids might be designed to achieve propulsive or rotational dynamics, and more generally for the extraction of work from active nematics.

BP 2.8 Mon 11:45 TOE 317

Structure and Dynamics of Active Polymer — •Sunil Pratap Singh — Indian Institute of Science Education and Research Bhopal, India, 462066

In this talk we are going to present structural and dynamical properties of a self-propelled filament using coarse-grained Brownian dynamics simulations. We consider two kinds of self-propulsion force on polymers, in case one force is applied tangent to the filament and in another model direction of active force is considered to be random. Case one shows that chain's stiffness and radius of gyration monotonically decrease. Moreover, the radius of gyration of the filament shows universal scaling for various bending rigidities with flexure number. In the latter model, where monomers are assumed to be active Brownian particle (ABP), displays a non-monotonic behaviour of end-to-end distance with activity strength. We will discuss here the role of many-body interactions on its structure and relaxation behavior. Additional we talk about the rheological behavior of chain under linear shear-flow. Our simulations reveal that active polymer's zero-shear viscosity varies in non-monotonic fashion with the active noise. More-importantly the viscosity decreases in the intermediate regime, that is followed by an increase in the more extensive Pe regime. We attribute the decrease of the zero-shear viscosity in the intermediate regime is due to many-body interactions among chain monomers.

BP 2.9 Mon 12:00 TOE 317

Pumping, Mixing, and Signal Transmission in Active Pores — •Goncalo Antunes[1,2,3], Paolo Malgaretti[1,2,3], Siegfried Dietrich[2,3], and Jens Harting[1,4] — [1]Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien (IEK–11), Forschungszentrum Jülich, Cauer Str. 1, 91058 Erlangen, Germany — [2]Max–Planck–Institut für Intelligente Systeme, Heisenbergstr. 3, 70569 Stuttgart, ,Germany — [3]IV. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [4]Department Chemie- und Bioingenieurwesen und Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Fürther Straße 248, 90429 Nürnberg, Germany

Much attention is currently being given to the problem of manipulating fluids at the microscale, with successful applications to fields such as 3D fabrication and biomedical research. An intriguing technique to manipulate fluid flows in a pore is diffusioosmosis. We show both numerically and analytically that a corrugated catalytic pore can act as a micropump even when it is fore-aft symmetric. This phenomenology is possible due to a spontaneous symmetry breaking which occurs when advection rather than diffusion is the dominant mechanism of solute transport. Relaxing the condition of Stokes flow leads to unsteady flow, and persistent oscillations with a tunable frequency appear. We further include the inverse chemical reaction that consumes solute and introduces an additional timescale. Finally, we find that the flow may lose its axial symmetry and hence promote mixing in the low Reynolds number regime.

BP 2.10 Mon 12:15 TOE 317

Interacting particles in an activity landscape — •Adam Wysocki[1], Anil Kumar Dasanna[1,2], and Heiko Rieger[1,2] — [1]Department of Theoretical Physics and Center for Biophysics, Saarland University, Saarbrücken, Germany — [2]INM-Leibniz Institute for New Materials, Saarbrücken, Germany

We study interacting active Brownian particles (ABPs) with a space-dependent swim velocity. We find that, although an equation of state exists, a mechanical equilibrium does not apply to ABPs in activity landscapes. The pressure imbalance originates in the flux of polar order across the interface between regions of different activity. An active-passive patch system is mainly controlled by the smallest global density for which the passive patch can be close packed. Below this density a critical point does not exist and the system splits continuously into a dense passive and a dilute active phase with increasing activity. Above this density and for sufficiently high activity the active phase may start to phase separate into a gas and a liquid phase caused by the same mechanism as motility-induced phase separation of ABPs with a homogeneous swim velocity.

BP 2.11 Mon 12:30 TOE 317

Active phase fluctuations of Chlamydomonas axonemes — •Abhimanyu Sharma[1], Benjamin M. Friedrich[2], and Veikko F. Geyer[1] — [1]B CUBE - Center for Molecular Bioengineering, TU Dresden, Dresden, Germany — [2]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany

Cilia and eukaryotic flagella generate periodic beat patterns by the activity of dynein motors. Earlier studies revealed active fluctuations in the ciliary beat arising presumably from small number fluctuations in the collective dynamics of the molecular motors that drive the beat. A theoretical model of the beating cilium as a system of coupled motors predicts that the fluctuations measured in terms of the quality factor of the oscillations scale with the number of beat-generating-motors.

To measure those fluctuations experimentally, we use in situ reactivated axonemes, the mechanical core of motile cilia isolated from the green alga Chlamydomonas. To modulate the number of motors in beating axonemes, we make use of motor mutants or partially extract molecular motors biochemically.

Using shape mode analysis and limit-cycle reconstruction, we characterize the phase fluctuations in the beat and report for the first time the relation between beat parameters and the motor number in Chlamydomonas axonemes. We experimentally infer scaling relations for the beat frequency, mean beat amplitude, and the quality factor. Further, using mass spectrometry, we identify specific dynein motors and infer their role in regulating the beat fluctuations.

BP 2.12 Mon 12:45 TOE 317

Lattice dynamics of pulsating active particles — •Alessandro Manacorda and Étienne Fodor — University of Luxembourg

Cells in epithelial tissues can drastically deform their shapes and volume giving rise to collective behavior such as size oscillation and wave propagation. These phenomena have a strinking impact in many biological contexts such as embryonic development, cardiac arrhythmias and uterine contraction.

The theoretical models describing the emergence of contractile waves so far consider the cells as motile particles, where activity is represented by self-propulsion; however this ingredient is questionable in dense systems where particles barely move. We therefore introduce a novel class of active matter where the activity is the ability to change an internal degree of freedom at the single-particle level e.g. particles' size. The collective behavior of active particles is investigated in a lattice model, where the interplay between pulsation and synchronization gives rise to emergent behavior such as wave propagation. Fluctuating hydrodynamic equations can be obtained from microscopic dynamics and their predictive power is shown in comparison with numerical simulations.

We highlight the minimal ingredients needed for the complex behavior above-mentioned and point out future directions in the growing field of pulsating active matter.

BP 3: Computational Biophysics I

Time: Monday 9:30–13:00 Location: BAR 0106

BP 3.1 Mon 9:30 BAR 0106

Elucidating the Binding Process of a Disordered Protein to a Membrane Containing Ionic Lipids via Atomistic Simulations: a Case Study of LKB1 — •Azadeh Alavizargar and Andreas Heuer — Institute of Physical Chemistry, University of Muenster, Corrensstr. 28/30, 48149 Muenster, Germany

Liver kinase LKB1 is a serine/threonine kinase, which apart from from playing a significant role in many biological processes such as cell proliferation and polarity, it functions also as a downregulator in tumors. In this work, we probe the significance of phosphatidic acid (PA) lipids as well as the poly-basic region for the binding of the C-terminus of the protein to the membrane, using molecular dynamics simulations. It was revealed that PA lipids are essential for the protein-membrane binding and that the mutation of the first three lysine residues does not abolish the binding. We specifically show the details of the protein-membrane binding at the atomic resolution using various amount of PA lipids in the membrane. Importantly, it was also found that the protein-membrane binding is dynamic and gives rise to structural changes of the protein as a result of the interaction and the accumulation of PA lipids in the membrane, which is beyond the accessible resolution in the corresponding experiments. Furthermore, we quantified the significance of each polar amino acid in the poly-basic region of the protein. These results provide important insights into the understanding and mechanism of the interaction of disordered proteins with membranes including ionic lipids.

BP 3.2 Mon 9:45 BAR 0106

Migration of oxygen in the human bc1 complex and the behavior of QH2 and Q cofactors inside it — •Katarina Kretschmer, Malena Kottke, and Ilia Solov'yov — Insitute of Physics, University of Oldenburg, Oldenburg, Germany

The dimeric bc1-complex embedded in the inner membrane of mitochondria is a relevant part of the respiratory chain in a mitochondrial cell of eukaryotes. Through different electron transfers that include oxidation and reduction reactions of the substrate molecules at the Qo- and Qi-site in this protein complex, it contributes to the metabolic system of the cell. Specifically, the complex facilitates proton transfers across the membrane to maintain an electrostatic potential, which is in turn used to drive ATP synthesis. This molecular machinery, however, is suspected to be a source of superoxide and is believed to be one of the factors in cellular aging.

Through molecular dynamics simulations, we have investigated the migration of molecular oxygen in the bc1-complex in order to identify possible reaction sites that could lead to superoxide formation. The investigation follows an earlier study of the bc1-complex from Rhodbacter capsulatus and reveals several important differences. Specifically, we investigate further into the behavior of the cofactors Ubiquinol (QH2) and Ubiquinone (Q) in both monomers in the bc1-complex and determine the oxygen diffusion pathways that could lead to the sites where O2 could be efficiently converted to superoxide, thereby disturbing the regular functioning of the bc1-complex.

BP 3.3 Mon 10:00 BAR 0106

On the road to cellular digital twins of in vivo tumors — •Eric Behle[1], Julian Herold[2], and Alexander Schug[1] — [1]NIC Research Group Computational Structural Biology, Jülich Supercomputing Centre, Jülich Research Center, Jülich, Germany — [2]Steinbuch Centre for Computing, KIT, Karlsruhe

To this day, cancer remains an insufficiently understood disease plaguing humanity. In particular, the mechanisms driving tumor invasion still require extensive study. Current investigations address collective cellular behavior within tumors, which leads to solid or fluid tissue dynamics. Furthermore, the extracellular matrix (ECM) has come into focus as a driving force facilitating invasion. To complement the experimental studies, computational models are employed, and advances in computational power within HPC systems have enabled the simulation of macroscopic tissue arrangements. We hereby present our work using Cells in Silico (CiS), a high performance framework for large-scale tissue simulation previously developed by us. CiS is capable of simulating tissues composed of tens of millions of cells, while accurately representing many physical and biological properties. Our ultimate aim is to build a cellular digital twin of an in vivo tumor. Unfortunately, current in vivo measurement methods lack the required resolution for directly parameterizing our simulations. Therefore, we aim to parameterize CiS via a bottom-up approach, utilizing experimental data from multiple in vitro systems. We focused our first studies on tumor spheroids, a main workhorse of tumor analysis. Towards this, we developed a novel method to compare spatial features of spheroids in 3D.

BP 3.4 Mon 10:15 BAR 0106

Resolving hierarchical interactions of proteins in phase-separated condensates by multi-scale simulations — •Lukas Stelzl[1,2,3], Kumar Gaurav[1,2,3], Xiaofei Ping[1,2,3], Arya Changiarath Sivadasan[1,2,3], René Ketting[3], and Dorothee Dormann[3,4] — [1]Institute of Physics, JGU Mainz, Germany — [2]Faculty of Biology, JGU Mainz, Germany — [3]IMB Mainz, Germany — [4]Institute of Molecular Physiology, JGU Main, Germany

Liquid-liquid phase separation and the resulting phase-separated condensates of proteins help to organize cellular processes in time and space. At same time, dysregulation of phase separation is implicated in the development of neurodegenerative diseases. Using particle-based multi-scale simulations we are elucidating how phase-separated condensates can provide for specific molecular recognition and thus cellular regulation and how this specificity is lost in diseases. With simulations we are elucidating how a hierarchy of interactions such as strong interactions of folded domains and weak and multivalent interactions between disordered regions of proteins determine phase behavior. With our multi-scale methods we can simulate condensates with atomic resolution and resolve molecular details of "sticker"-"sticker" interactions, their kinetics and how these provide for specific recognition and cellular function. We also show how mutations and biochemical modifications can shift the conformational equilibria of proteins and their interactions in phase-separated condensates and favor the formation of toxic aggregates in neurodegenerative diseases.

Invited Talk BP 3.5 Mon 10:30 BAR 0106

Resolving gating and allosteric modulation in ion channels through simulations and small-angle neutron scattering — •Erik Lindahl — Dept. Biophysics & Biochemistry, Science for Life Laboratory, Stockholm University

Pentameric ligand-gated ion channels (pLGICs) perform electrochemical signal transduction in organisms ranging from bacteria to humans. In addition to their normal gating cycle, pLGICs are highly sensitive to allosteric modulation where small compounds such as barbiturates, benzodiazepines or alcohols influence the gating kinetics by binding in separate sites, either in the transmembrane or extracellular domain. Despite a wealth of new experimental structures, it has been challenging to understand the gating kinetics, in particular since the channels rapidly undergo transitions to a desensitized nonconducting state rapidly after opening. I will present our recent combined experimental and computational work on a number of prokaryotic and eukaryotic pLGICs from the team, and how we are trying to combine low-resolution experimental techniques such as SANS (small-angle neutron scattering) with simulations to model channels under realistic conditions. In addition, I will show how we have been able to resolve structures in all separate functional states, their state-specific interactions with lipids, and not least how we are beginning to understand the properties of the desensitized state.

15 min. break

BP 3.6 Mon 11:15 BAR 0106

Clustering Molecular Dynamics Trajectories using Density and Flux — •Jayashrita Debnath[1] and Gerhard Hummer[1,2] — [1]Max Planck Institute of Biophysics, Frankfurt am Main, Germany — [2]Goethe University, Frankfurt am Main, Germany

Molecular dynamics (MD) simulations are a powerful tool for studying a wide range of molecular systems and processes, with applications ranging from materials science to biology and medicine. Analyzing these simulations often involves finding a low-dimensional representation of the trajectory data and clustering the sampled configurations into kinetically relevant metastable states. The steady growth in the time and length scales of MD simulations, and in the complexity of their molecular systems, necessitates the development of new analysis

tools that do not rely entirely on chemical or physical intuition. Here, we propose a neural network based unsupervised algorithm that can identify states using the static and dynamic information encoded in the trajectories. The network identifies metastable states by modeling a probability distribution of the data in a reduced dimensional space and learns the state boundaries by minimizing the flux between states. Furthermore, it can learn the optimal number of states from single long equilibrium trajectories or multiple short ones. After demonstrating the effectiveness of this method for a toy potential, we apply it to trypsin-benzamidine unbinding as a model of drug binding kinetics, to and folding-unfolding transitions of the villin headpiece subdomain.

BP 3.7 Mon 11:30 BAR 0106

Enhancing Traction-Force Microscopy with Machine Learning — •Felix S. Kratz, Lars Möllerherm, and Jan Kierfeld — TU Dortmund University, Germany

Traction patterns of adherent cells provide important information on their interaction with the environment, cell migration or tissue patterns and morphogenesis. Traction Force Microscopy is a method aimed at revealing these traction patterns for adherent cells on engineered substrates with known constitutive elastic properties from deformation information obtained from substrate images. Conventionally, the substrate deformation information is processed by numerical algorithms of varying complexity to give the corresponding traction field via solution of an ill-posed inverse elastic problem. We explore the capabilities of a deep convolutional neural network as a computationally more efficient and robust approach to solve this inversion problem. We develop a general purpose training process based on collections of circular force patches as synthetic training data, which can be subjected to different noise levels for additional robustness. The performance and the robustness of our approach against noise is systematically characterized for synthetic data, artificial cell models and real cell images, which are subjected to different noise levels. A comparison to state-of-the-art Bayesian Fourier transform traction cytometry reveals the precision, robustness, and speed improvements achieved by our approach, leading to an acceleration of Traction Force Microscopy methods in practical applications.

BP 3.8 Mon 11:45 BAR 0106

Finding pathways in molecular dynamics simulations using machine learning and graph methods — •Steffen Wolf[1], Miriam Jäger[1], Victor Tänzel[1], Simon Bray[1,2], Matthias Post[1], and Gerhard Stock[1] — [1]Biomolecular Dynamics, Institute of Physics, University of Freiburg, 79104 Freiburg, Germany — [2]Bioinformatics Group, Institute of Informatics, University of Freiburg, 79110 Freiburg, Germany

Understanding the mechanisms of biomolecular systems and complexes, e.g., of protein-ligand (un)binding, requires the understanding of paths such systems take between metastable states. In MD simulation data, paths are usually not observable per se, but need to be inferred from simulation trajectories. Here we present novel approaches to cluster trajectories according to similarities. These approaches include neighbor-nets allowing to correct for input data ambiguity [1] and an unsupervised learning approach employing only a single free parameter [2]. We demonstrate how such clusters of trajectories correspond to pathways, and how the approaches help in the identification of reaction coordinates for a considered process. Last, we present a theoretical framework how potentials of mean force can be calculated for individual pathways, and how these potentials and kinetics along paths can be combined into a comprehensive complete free energy profile and process kinetics.

[1] Bray, S., Tänzel, V. & Wolf, S. J. Chem. Inf. Model. 62, 4591-4604 (2022). [2] Diez, G., Nagel, D. & Stock, G. J. Chem. Theory Comput. 18, 5079-5088 (2022).

BP 3.9 Mon 12:00 BAR 0106

Artificial Intelligence for Molecular Mechanism Discovery — •Hendrik Jung[1], Roberto Covino[2], A Arjun[3], Christian Leitold[4], Peter G Bolhuis[3], Christoph Dellago[4], and Gerhard Hummer[1] — [1]Max Planck Institute of Biophysics, Frankfurt, Germany — [2]Frankfurt Institute for Advanced Studies, Frankfurt, Germany — [3]University of Amsterdam, Amsterdam, The Netherlands — [4]University of Vienna, Vienna, Austria

We present a machine learning algorithm to extract the mechanism of collective molecular phenomena from computer simulations. The algorithm combines transition path sampling (TPS), deep learning (DL), and statistical inference to simultaneously enhance the sampling and understanding of complex molecular reorganizations without human intervention. TPS is a Markov Chain Monte Carlo method in trajectory space that samples the rare transition trajectories connecting meta-stable states. In our algorithm a DL model is selecting the configurations from which the new trial trajectories are generated using shooting moves, i.e., the trajectories are propagated according to the physical model of the simulated system. By iteratively training on the outcomes of the shooting moves, the model simultaneously increases the efficiency of the rare-event sampling and gradually reveals the underlying mechanism of the transition. In a second step we distill the knowledge about the transition encoded in the DL model into a simplified mathematical expression. With this algorithm we study a diverse set of molecular systems ranging from the association of ions in solution to the oligomerization of a transmembrane alpha helix dimer.

BP 3.10 Mon 12:15 BAR 0106

MD simulations of *n*-alkanes in a phospholipid bilayer: CHARMM36 vs. Slipids — •Anika Wurl and Tiago Ferreira — Institute of Physics, Martin-Luther Universität Halle-Wittenberg

The incorporation of *n*-alkanes into phospholipid bilayers is a convenient starting point for studying the molecular behavior of linear, (purely) hydrophobic molecules in lipid membranes. Here, we perform atomistic molecular dynamics simulations using two state-of-the-art lipid force fields, CHARMM36 [1] and Slipids [2], to systematically investigate how the miscibility of n-alkanes in dipalmitoylphosphatidylcholine (DPPC) bilayers depends on alkane chain length. The two force fields show a distinct behavior: Slipids simulations predict an effect of chain length on miscibility, while for CHARMM36 simulations this is not the case for the alkanes studied. A comparison with ^{2}H NMR spectra shows that the accuracy of the two force fields is dependent on alkane length. CHARMM36 performs well for the shorter chains, while Slipids models the longer alkanes better. Slipids chains are more flexible, due to reduced electrostatic 1-4 interactions compared to CHARMM36. By scaling these 1-4 interactions, CHARMM36 can be adapted to model longer alkanes and lipid acyl tails better. The presented results are of general interest for future studies of other long and flexible hydrophobic molecules inside lipid membrane environments, and show that *n*-alkane/lipid mixtures should be taken into account for optimization of force fields designed to model lipid membranes. [1] Jämbeck et al.; *J Phys Chem B* 2012, 116, 3164-3179 [2] Klauda et al.; *J Phys Chem B* 2010, 114, 7830-7843

BP 3.11 Mon 12:30 BAR 0106

Scission criteria upon proteins X-ray absorption — •Carlos Ortiz-Mahecha[1], Lucas Schwob[2], Sadia Bari[2], and Robert Meissner[1,3] — [1]Technische Universität Hamburg, Hamburg, Germany — [2]Deutsches Elektronen-Synchrotron, Hamburg, Germany — [3]Helmholtz-Zentrum Hereon, Geesthacht, Germany

Dynamic protonation in a protein lead to conformational changes which could be studied by challenging near-edge X-ray absorption mass spectrometry (NEXAMS) experiments and computationally expensive quantum mechanical (QM) calculations. Less demanding assessment is essential for interpreting the underlying electronic density changes in proteins. Those density changes in the amino-acid (AA) non-covalent environment are evaluated by *in-silico* X-ray spectra and their chemical-physical properties by the pair interaction energy decomposition analysis (PIEDA) method. In order to represent a protein X-ray absorption spectra as a summation of their smaller protein fragments X-ray spectra, we first assess its electronic neighboring influence to establish a scission criteria. For that, we propose a pattern involving the change of excited-state transition energy probability in a two-body AA localized density population and the charge transfer energy change from PIEDA as a function of the non-covalent interaction distance. In this way using this criteria, the X-ray absorption spectra of proteins could potentially be represented as a composition of X-ray spectra of their smaller fragments, which would be computationally more efficient.

BP 3.12 Mon 12:45 BAR 0106

Fluid defomable surfaces, the influence of surface viscosity in fluid membranes — Veit Krause and •Axel Voigt — Institute of Scientific Computing, Technische Universität Dresden, Germany

We consider a fluid-solid duality of membranes, with in-plane fluid properties and out-of-plane solid (bending) properties. In such systems any tangential flow induces shape deformationas and any change in morphology induces tangential flow. This numerically challanging surface problem is solved by surface finite elements and we explore

the dynamics towards equilibrium states in various settings, ranging from transitions from biconcave to dumbell shapes, coarsening of two-component surface fluids under the influence of curvature and wrinkling in fluid membranes.

BP 4: Tissue Mechanics I

Time: Monday 15:00–17:30 Location: BAR Schö

BP 4.1 Mon 15:00 BAR Schö

Nonlinear and active rheology of cell tissues — •Charlie Duclut[1,2], Joris Paijmans[2], Mandar M. Inamdar[3], Carl D. Modes[4], and Frank Jülicher[2] — [1]Laboratoire Physico-Chimie Curie, Paris, France — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Indian Institute of Technology Bombay, Mumbai, India — [4]Max Planck Institute for Molecular Cell Biology and Genetics, Dresden, Germany

Tissues are assemblies of large numbers of cells which form a soft active material. In amorphous solids as in tissues, neighbour exchanges (or T1 transitions) can relax local stresses and allow the material to flow. In tissues, in addition to these passive events, energy consumption at the microscopic level allows cells to perform active neighbour exchanges that can shape the tissue into a prescribed geometry. In my talk, I will consider an anisotropic vertex model to study T1 rearrangements in polygonal cellular networks. I will consider two different physical realizations of the active anisotropic stresses, that can be both observed in experiments: (i) anisotropic bond tension and (ii) anisotropic cell stress. Interestingly, the two types of active stress lead to patterns of relative orientation of T1 transitions and cell elongation that are different. Using the lens of a continuum description of the tissue as an anisotropic active material, I will discuss the energetics of the dynamic tissue and express the energy balance in terms of internal elastic energy, mechanical work, chemical work and heat. This allows us to define active T1 transitions that can perform mechanical work while consuming chemical energy.

BP 4.2 Mon 15:15 BAR Schö

Hydraulic and osmotic control of lumen coarsening — •Mathieu Le Verge Serandour[1,2] and Hervé Turlier[2] — [1]School of Natural Sciences, Technical University of Munich, Germany — [2]Center for Interdisciplinary Research in Biology, Collège de France, PSL Research University, Paris, France

The blastocoel formation is a keystone in the morphogenesis of the pre-implantation mammalian embryo, yet the physical mechanism for its emergence remained unclear. The blastocoel is a fluid-filled cavity (or lumen) that positions the first axis of symmetry of the embryo. We showed that, in the mouse embryo, the blastocoel results from micron-sized lumens, nucleating at the adhesive basolateral side of embryonic cells and coarsening in a process akin to Ostwald ripening. We investigate the collective dynamics of a one-dimensional chain of lumens as a minimal model for the blastocoel formation, taking the osmotic effects into account. We include the permeation of water and osmolyte through the cellular membrane. We show that the coarsening of the chain is reminiscent of dewetting films, with a scaling law for the number of lumens controlled by a screening length associated with water permeation, while the influence of osmotic inhomogeneities remains limited. Finally, we consider active osmolyte pumping that may rescue the chain from collapse. We find a new scaling law controlled by active pumping emerging from the coalescence of lumens, which may also direct the position of the final lumen.

BP 4.3 Mon 15:30 BAR Schö

Mechanical Properties of the Premature Lung — •Jonas Naumann[1], Nicklas Koppe[1], Ulrich Thome[2], Mandy Laube[2], and Mareike Zink[1] — [1]Research Group Biotechnology & Biomedicine, Peter Debye Institute for Soft Matter Physics, Leipzig University, 04103 Leipzig, Germany — [2]Center for Pediatric Research Leipzig, Department of Pediatrics, Division of Neonatology, Leipzig University, 04103 Leipzig, Germany

Premature infants are often reliant on mechanical ventilation to survive. However, prolonged ventilation and associated mechanical stress may cause subsequent pulmonary diseases of the immature lung. To study the mechanical properties of fetal rat lungs on macroscopic scale, we performed rheology experiments under compression and tension using different velocities. Fetal lung tissue showed a hyperelastic behavior and became significantly stiffer with increasing deformation velocities. In fact, fetal lung tissue under compression showed clear viscoelastic features even for small strains. A higher Young's modulus of fetal lungs compared to adult controls clearly pointed towards altered tissue characteristics. In addition, the influence of a hydrostatic pressure difference on the electrophysiology of primary fetal distal lung epithelial cells was investigated on microscopic scale. We observed a strong impact of hydrostatic pressure on the activity of the epithelial sodium channel and the sodium-potassium pump. Vectorial sodium transport, crucial for alveolar fluid clearance, was significantly impaired.

BP 4.4 Mon 15:45 BAR Schö

'Forcing' changes in health and disease: New access into bioengineered skeletal muscle mechanics for preclinical screening — •Arne Hofemeier[1,2], Till Muenker[2], Mariam Ristau[2], Timo Betz[2], and Wolfram Zimmermann[1] — [1]University Medical Center, Göttingen, Germany — [2]Third Institute of Physics, Göttingen, Germany

Mechanical properties of skeletal muscles are tightly related to proper functionality, which makes experimental access to the biomechanics of skeletal muscle tissue essential to advance our understanding of muscle function, development and disease. Recently devised in vitro culture systems allow for raising 3D muscle tissues using single cells from patients. However, these systems are inherently incompatible with high resolution microscopy and precise mechanical in-plate measurements. Here, we present a new chamber design that allows real-time high resolution 3D microscopy and non-invasive quantification of global contractile forces and tissue tension during muscle formation. Surprisingly, we found that bioengineered muscles, derived from patients suffering from Duchenne muscular dystrophy, develop under higher tension although they appear weaker upon stimulation. Duchenne is caused by loss of a membrane linker protein, dystrophin, which we therefore dedicate an important novel role as a molecular tension sensor. Testing an individualized gen therapy for a subset of Duchenne patients, we were able to demonstrate that not just the contractile strength of the bioengineered muscles was restored, but also the elevated tissue tension was decreased again.

15 min. break

BP 4.5 Mon 16:15 BAR Schö

Harnessing active viscoelasticity for synthetic epithelial morphogenesis — •Nimesh Ramesh Chahare[1,2], Adam Ouzeri[2], Tom Golde[1], Thomas Wilson[1,3], Pere Roca-Cusachs[1], Marino Arroyo[2,3], and Xavier Trepat[1,4] — [1]Institute for Bioengineering of Catalonia, Barcelona, Spain — [2]Universitat Politècnica de Catalunya, Barcelona, Spain — [3]Centre Internacional de Mètodes Numèrics en Enginyeria, Barcelona, Spain — [4]Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain

Epithelial sheets are active viscoelastic materials that form specialized 3D structures suited to their physiological roles, such as branched alveoli in the lungs, tubes in the kidney, and villi in the intestine. How epithelial shape arises from active viscoelasticity and luminal pressure remains poorly understood. Here we developed a microfluidic setup to engineer 3D epithelial tissues with controlled shape and pressure. Through this approach, we subject the tissues to a range of lumen pressures at different rates and probe the relation between strain and tension in different regimes. Slow pressure changes relative to the timescales of actin dynamics allow the tissue to accommodate large strain variations. However, under sudden pressure reductions, the tissue buckles and folds to store excess tissue area. This behavior is well captured by a 3D computational model that incorporates the turnover, viscoelasticity, and contractility of the actomyosin cortex. Informed by this model, we harness the active behavior of the cell cortex to pattern epithelial folds by rationally directed buckling. Our study establishes a new approach to engineering epithelial morphogenetic events.

BP 4.6 Mon 16:30 BAR Schö

Continuum Mechanics of Cell Intercalation in *Tribolium* —

•Maryam Setoudeh[1,2,3] and Pierre A. Haas[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstraße 108, 01307 Dresden, Germany — [3]Center for Systems Biology Dresden, Pfotenhauerstraße 108, 01307 Dresden, Germany

Deformations of tissues during development often involve cell intercalations and cell neighbour exchanges, but a general continuum description of such plastic rearrangements in tissues is still lacking.

Here, we combine morphoelasticity and plasticity theory to develop a continuum framework of tissue mechanics combining cell intercalations, intrinsic deformations such as tissue contraction, and elastic deformations of the tissue.

We apply our theory to the development of the beetle *Tribolium* [1] during which a layer of cells, the serosa, closes over the embryo. Cells deintercalate from the rim of the serosa into its bulk, thus reducing the number of cells at the boundary and closing the serosa. This is associated with actomyosin contraction at the rim of the serosa [1].

We model this process by the axisymmetric closure of a circular hole in a flat elastic sheet contracting near the hole. Our analytical and numerical results show how intercalation reduces the contraction required for serosa closure and hint at the importance of an additional force exerted by the embryo at the rim of the serosa.

[1] Jain *et al.*, Nat. Commun. **11**, 5604 (2020)

BP 4.7 Mon 16:45 BAR Schö

Tracking and comprehending single cell dynamics in Drosophila dorsal closure using machine learning — •Daniel Härtter[1,3], Yuxi Long[2], Janice Crawford[2], Daniel P. Kiehart[2], and Christoph F. Schmidt[1] — [1]Department of Physics and Soft Matter Center, Duke University, USA — [2]Department of Biology, Duke University, USA — [3]Department of Pharmacology and Toxicology, Göttingen University Medical Center

Dorsal closure in Drosophila melanogaster embryos is a key model system for cell sheet morphogenesis and wound healing. We pursue a data-driven approach to understand the emergence of organized behavior on tissue level from the stochastic dynamics of single cells across scales. We developed DeepTissue, a deep-learning-based algorithm to automatically and robustly detect and temporally track various single cell features: cell shapes, cell junction lengths, myosin intensities, and tissue topology. Epithelial cells in dorsal closure exhibit oscillations and contribute to progressive cell sheet movements, while showing a large variability in individual shapes, dynamics, and fates. Based on high-quality multi-parametric trajectories of 1000s of single cells, we use unsupervised machine learning techniques to detect and classify behavioral and structural phenotypes. Further we study how the behavior of single cells throughout closure is driven by deterministic and/or stochastic factors, with the aim to predict singular cell ingression events.

BP 4.8 Mon 17:00 BAR Schö

The role of intermediate filaments in stress resistance in 3D epithelial structures — •Tom Golde[1], Marco Pensalfini[2], Nimesh Chahare[1], Marino Arroyo[1,2], and Xavier Trepat[1,3,4] — [1]IBEC, Barcelona, Spain — [2]UPC, Barcelona, Spain — [3]UB, Barcelona, Spain — [4]ICREA, Barcelona, Spain

The safety belt hypothesis states that IFs are protecting cells from large and rapid deformations. However, typical experiments for stretching epithelial tissues only reach maximum strains of around 0.3. We developed a microfluidic device where an epithelial monolayer is grown on a porous surface with circular low adhesion zones. Upon applying hydrostatic pressure, the monolayer delaminates into a spherical cap (dome), generating tissue strains of more than 1 while individual cells are stretched up to strains of 9. We can image these 3D epithelial domes with high resolution, determine the tissue tension via Laplace law, and control the rate of inflation and deflation.

Using this approach with MDCK cells, we observed a striking reorganization of the keratin IF rim-and-spoke network into a central knot with thick, radially oriented bundles. Previous results by us and others hereby indicate a crucial role of actin-IF interactions. To better understand the mechanical principles of such transitions, we developed a multiscale computational model that simulates the interactions of keratin IFs with the nucleus, desmosomes, and the actin cortex. Combining experiments and simulations, we can now conclusively test the safety belt hypothesis in controlled and unparalleled large 3D tissue deformations

BP 4.9 Mon 17:15 BAR Schö

Instabilities in hexanematic models of epithelia — •Josep-Maria Armengol-Collado, Livio Carenza, and Luca Giomi — Instituut-Lorentz, Leiden Institute of Physics, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands

Epithelial tissues, whose study remain fundamental to understand processes such as cancer progression, have revealed to exhibit multiscale orientational order. While the large scale dynamics is ruled by the nematic symmetry, hexatic order instead controls the behaviour of small clusters of cells. By considering a hydrodynamic approach, we investigate the stability of hexanematic liquid crystals identifying the role of activity and flow alignment in the generation of spontaneous flows, which also reflect the interplay between different length scales. We finally address possible consequences when confining such a fluid in a channel, connecting this phenomenology with recent observations of metastatic cell invasion.

BP 5: Focus Session NanoAgents

Time: Monday 15:00–17:30 Location: TOE 317

Invited Talk BP 5.1 Mon 15:00 TOE 317

Repurposing nucleic acids as high-resolution force sensors: From fundamental mechanotransduction to translational biophysics — •Khalid Salaita — Emory University, Department of Chemistry, Atlanta, Georgia, USA

Cells are highly dynamic structures that are constantly converting chemical energy into mechanical work to pull and push on one another and on their surroundings. These pulls and pushes are mediated by tiny molecular forces at the scale of tens of piconewtons. For context, 7 pN applied a distance of 1 nm is ~1 kcal/mol. Nonetheless, these forces can have profound biochemical consequences. For example, the rapidly fluctuating forces between immune cells and their targets can drastically tune immune response and function. Despite the importance of mechanics there are limited methods to study forces at the molecular scale and particularly within living cells.

In this talk, I will discuss my group's efforts at addressing this gap in knowledge by developing tools to map the molecular forces applied by cells. I will describe the development of a suite of DNA tension probes which offer significant improvements in S/N and lead to enhanced spatial and temporal resolution. I will also describe a series of force-triggered reactions that enable signal amplification. Fluorescence polarization spectroscopy and super-resolution imaging offer the highest resolution maps of cell traction forces reported to date. Finally, armed with these new tools, I will describe the advent of translational mechanobiology where we predict the bleeding risk in patients by measuring the mechanical activity of their platelet adhesion receptors.

BP 5.2 Mon 15:30 TOE 317

Remodelling DNA filaments for bottom-up synthetic biology — •Maja Illig[1], Kevin Jahnke[1,2], Marlene Scheffold[1], Hauke Drechsler[3], Stefan Diez[3], and Kerstin Göpfrich[1] — [1]MPI for Medical Research, Heidelberg, Germany — [2]Harvard University, School of Engineering and Applied Sciences (SEAS), Cambridge, MA, USA — [3]TU Dresden, Center for Molecular Bioengineering (B CUBE), Dresden, Germany

The control of filamentous cytoskeletal systems is one of the dedicated aims of bottom-up synthetic biology to engineer self-dividing synthetic cells and equip them with mechanical cell-to-cell communication pathways. A molecular engineering approach to achieve specific functionality from the nanoscale to the microscale requires programmability in order to design self-assembly.

This work reinforces how DNA nanotechnology paves the way to create biocompatible nanostructures that can mimic cellular entities. Here, we demonstrate the remodelling of entirely synthetic filaments

made from DNA nanotubes: (i) Towards bottom-up synthetic cell division, we can rationally design a ring structure made from bundled filaments. We can control the ring formation by engineering of a synthetic crosslinking peptide and we further constrict the ring diameter by external triggers. (ii) Towards mechanotactic synthetic cells, a transmembrane signalling pathway enables the reconfiguration of the cytoskeleton made from DNA filaments. The stimulus-induced clustering of transmembrane entities results in mechanical remodelling of the internal DNA cytoskeleton (Jahnke, Illig et al. Biorxiv 2022).

BP 5.3 Mon 15:45 TOE 317

Einfluss von Kohlenstoff-Nanoteilchen auf die Funktion von Lysosomen — •Carla Sprengel, Cathrin Nollmann, Lena Berning, Thomas Lenz, Björn Stork und Thomas Heinzel — Heinrich-Heine-Universität Düsseldorf

Die Verwendung von Nanopartikeln als Wirkstoffträger in Drug Delivery Systemen gewinnt besonders bei der Tumortherapie an Bedeutung. Die zielgenaue Medikamentenfreisetzung in pathologischen Zellen könnte bei gleichbleibender therapeutischer Wirkung starke Nebenwirkungen durch Schädigung gesunder Zellen vermeiden. Kohlenstoff-Nanopartikel (CNDs) eignen sich aufgrund ihrer Fluoreszenzeigenschaften, geringen Zytotoxizität und Möglichkeit zur Funktionalisierung besonders gut als Carrier für ein solches Drug Deliver System. Durch die Fluoreszenz der CNDs im blauen Bereich nach UV-Anregung können die CNDs in Zellen nachgewiesen werden und auf zellulärer Ebene lokalisiert werden. Bisherige Untersuchungen zeigen, dass die CNDs über Endozytose in die Zelle aufgenommen und in den Endosomen und Lysosomen angelagert werden. Da wichtige metabolische Prozesse wie die Autophagie abhängig von Lysosomen sind, werden die Auswirkungen der CNDs auf diese lysosomalen Prozesse mittels verschiedener Methoden untersucht und diskutiert.

BP 5.4 Mon 16:00 TOE 317

Aufnahme von Kohlenstoff-Nanopartikeln in humane AML-Zellen im Vergleich zu primären hämatopoetischen Zellen — •Cathrin Nolllmann[1], Thomas Heinzel[1] und Rainer Haas[2] — [1]Institut für Physik der kondensierten Materie, Heinrich-Heine-Universität, Düsseldorf, Deutschland — [2]Klinik für Hämatologie, Onkologie und Klinische Immunologie, Universitätsklinikum Düsseldorf, Deutschland

Kohlenstoff-Nanopartikel (CNDs) sind eine vielversprechende Klasse von Nanopartikeln. Diese kohlenstoffbasierten, nanometergroßen Partikel bieten ein breites Spektrum potenzieller biomedizinischer Anwendungen wie Bioimaging, Krebsdiagnostik und Drug-Delivery. Im Zusammenhang mit Drug Delivery ist eine selektive Aufnahme durch maligne Zellen entscheidend. Unser Ziel war es zu untersuchen, ob es ein unterschiedliches Aufnahmeverhalten von AML-Zellen im Vergleich zu primären hämatopoetischen Zellen gibt. Dazu wurden aus Zitronensäure und Diethylentriamin hergestellte CNDs 24 Stunden lang mit Zellen von fünf Patienten mit de novo AML und primären hämatopoetischen Zellen von drei gesunden Spendern inkubiert. Die differentielle Aufnahme der CNDs wurde mittels Durchflusszytometrie und monoklonalen Antikörpern untersucht. [1]

[1] C. Nollmann et al., Uptake of carbon nanodots into human AML cells in comparison to primary hematopoietic cells, RSC Adv., (11), pp. 26303-26310, 2021.

15 min. break

BP 5.5 Mon 16:30 TOE 317

DNA origami agents for the efficient treatment of solid tumors — •Johann Moritz Weck[1], Merve-Zeynep Kesici[1], Cornelia Monzel[2], and Amelie Heuer-Jungemann[1] — [1]Max Planck Institut für Biochemie, Am Klopferspitz 18, 82152 Martinsried — [2]Heinrich Heine Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf

We previously used DNA origami as a platform to pre-cluster Fas ligands (FasL) of the tumor necrosis factor receptor superfamily (TNFRSF) with nanometer precision in varying patterns and presented those to HeLa cells in a 2D cell culture model. We found up to a 100x increase of potency upon pre-clustering FasL in hexagonal geometries, a high sensitivity towards inter-ligand distance and a dependency on linker rigidity. In order to use this knowledge for the advancement of TNRSF ligand-based therapeutics, we investigated the interactions of DNA origami nanoagents with solid tumors. Certain aspects of cancer cell biology, such as the complex biological environment of solid tumors cannot be efficiently simulated in regular 2D cell culture systems. Using a 3D tumor spheroid model, we here show that FasL-DNA origami nanoagents are able to strongly affect the growth of 3D tumor spheroids. Partial dissolution of 3D tumoroids is observed after exposure to the nanoagents. We provide insights into DNA origami tumor spheroid penetration ability as well as a threshold like behavior of signaling initiation, and design rules for nanomaterial based therapeutics.

BP 5.6 Mon 16:45 TOE 317

Monitoring the Switching dynamics of Photolipid Membranes with Plasmonic Nanorods — •Jinhua Zhang, Francis Schuknecht, Ludwig Habermann, Alexander Pattis, Stefanie Pritzl, and Theobald Lohmüller — Chair for Photonics and Optoelectronics, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität, Königinstraße 10, 80539 Munich, Germany

Photoswitchable lipids (i.e. photolipids) are intriguing nanoagents for controlling lipid membrane properties with light. However, analyzing the switching dynamics in a single lipid bilayer locally and in situ is challenging due to a lack of sensitive tools for detecting the very small changes in membrane thickness (< 1 nm). Here, we demonstrate a new approach to monitor the photoisomerization of photolipid membranes on the nanoscale via plasmonic sensing.

In our experiment, gold nanorods are deposited on a glass substrate and coated with a supported photolipid bilayer. The photosensitive azobenzene group in the lipid tails is switched between a trans and cis form by an illumination sequence with UV and blue light, while scattering spectra of individual nanorods are simultaneously measured. We find that the photoisomerization process of azobenzene leads to a reversible shift of the nanorod's plasmon resonance over many switching cycles. Our study shows that single nanorods may thus be used as sensitive probes to study isomerization dynamics and photostationary states of photolipid bilayer membranes within nanoscale environments.

BP 5.7 Mon 17:00 TOE 317

Bio-inspired Magnetic Nanoprobes For Subcellular Manipulation Studies in Single Cells — •Andreas Neusch[1], Iuliia Novoselova[1], Liesa Zitzke[1], Sarah Sadik[1], Michael Farle[2], Ulf Wiedwald[2], and Cornelia Monzel[1] — [1]Heinrich-Heine-University, Düsseldorf — [2]University of Duisburg-Essen, Duisburg

Probing and manipulating biological functions requires tools to target and modify the proteins involved in the respective process. In recent years Magnetogenetics emerged as an approach where magnetic nanoparticles (MNPs) and external magnetic fields are used to realize such manipulation (Lisse et al., Adv. Mater., 29, 1700189 (2017)). The advantages of this combination lies within the deep tissue penetration of magnetic fields and the possibility to apply stimuli on nanoscales leading to spatial redistribution, force application, or heat generation of proteins. However, a precise active perturbation requires MNPs to be monodisperse, biocompatible, tunable with regard to their magnetic properties, as well as exhibiting a modifiable molecular shell (Monzel et al., Chem. Sci. 8, 7330-7338 (2017)). Here, we synthesize a bioinspired semisynthetic MNP - Magnetoferritin (MFt) -, which fulfils these demands. MFt is based on the globular iron storage protein complex ferritin that converts iron ions to a ferrihydrite core but can be synthetically loaded with a magnetic iron oxide core (Novoselova et al., Nanomaterials, 11, 2267 (2021)). MFt was chemically, physically and magnetically characterized both in vitro and in vivo. We demonstrate how MFt can be used to target proteins on living cells as well as to spatially manipulate MFts in a single cell environment.

BP 5.8 Mon 17:15 TOE 317

Precise micro-manipulations via multiplexed feedback-controlled thermoviscous flows — •Elena Erben[1], Nicola Maghelli[1], Weida Liao[2], Antonio Minopoli[1], Eric Lauga[2], and Moritz Kreysing[1] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]DAMTP, University of Cambridge, UK

Methods for precise micro-manipulation are highly relevant for many problems in biological research such as cell patterning and controlled droplet fusion. Thermoviscous flows [1] hold great potential for manipulations in biological systems since they can be induced optically and enable non-invasive in-vivo perturbations [2]. Recently, we developed a novel optofluidic manipulation method based on feedback-controlled thermoviscous flows. This technique facilitates the automatic positioning of a single micro-particle, with a precision of up to 24 nm [3]. Our approach can be multiplexed to the parallel manipulation of multiple particles, thus facilitating dynamic micropatterning. Furthermore, we

found that positioning of multiple particles can be greatly accelerated by leveraging highly complex flow patterns that result from multiplexing. We anticipate that combining our approach with elaborate theoretical modelling will increase the precision and speed of this manipulation method even more, facilitating translation onto applications in the life sciences and beyond.

[1] Weinert et al. Phys. Rev. Lett. 2008; [2] Mittasch et al. Nat. Cell Biol. 2018; [3] Erben et al. Opt. Express 2021.

BP 6: Bacterial Mechanics

Time: Monday 15:00–17:15 Location: BAR 0106

BP 6.1 Mon 15:00 BAR 0106

Antigenic variation modulates attractive forces between bacteria and affects antibiotic tolerance — •Isabelle Wielert[1,3], Sebastian Kraus-Römer[1,3], Paul Higgins[2,3], and Berenike Maier[1,3] — [1]Institute for Biological Physics, University of Cologne, Germany — [2]Institute for Medical Microbiology, Immunology and Hygiene, University of Cologne, Germany — [3]Center for Molecular Medicine Cologne

Type 4 pili (T4P) are multifunctional surface exposed polymers involved in adhesion, force generation, surface motility, aggregation and act as major antigens. During antigenic variation, the human pathogen Neisseria gonorrhoeae varies the primary structure of the pilin, the major subunit of the T4P fibre, to escape from immune surveillance. But it is unclear how pilin antigenic variation impacts other T4P functions. We addressed this question by replacing the pilin of a laboratory strain by pilins from various clinical isolates. By performing dual laser trap experiments, we found that the pilin variant strains clustered into two groups with different attractive forces. Variants with interaction forces exceeding 40 pN formed colonies while weakly interacting bacteria retained a planktonic lifestyle. All pilin variants supported surface motility, yet the planktonic variants moved faster. Previous studies indicated that bacterial aggregation results in higher tolerance against antibiotic treatment. To test whether pilin antigenic variation affects tolerance, we carried out bacterial survival assays and showed that indeed colony-forming variants are more tolerant. We conclude that pilin variation enhances bacterial fitness beyond immune escape.

BP 6.2 Mon 15:15 BAR 0106

Stress anisotropy in confined populations of growing rods — Jonas Isensee[1,2], Lukas Hupe[1,2], Ramin Golestanian[1,2,3], and •Philip Bittihn[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, Göttingen University — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, UK

A central feature of living matter is its ability to grow and multiply. The mechanical activity associated with growth produces both macroscopic flows shaped by confinement, and striking self-organization phenomena, such as orientational order and alignment, which are particularly prominent in populations of rod-shaped bacteria due to their nematic properties. However, how active stresses, passive mechanical interactions and flow-induced effects interact to give rise to global alignment patterns remains elusive. Here, we study in silico colonies of growing rod-shaped particles confined in channel-like geometries. A spatially resolved analysis of the stress tensor reveals a strong relationship between near-perfect alignment and an inversion of stress anisotropy for particles with large length-to-width ratios. In quantitative agreement with an asymptotic theory, strong alignment can lead to a decoupling of active and passive stresses parallel and perpendicular to the growth axis, respectively. We demonstrate the robustness of these effects to perturbations and for weaker confinement. Our results illustrate the complexity arising from the inherent coupling between nematic order and active stresses in growing active matter, modulated by geometric and configurational constraints due to confinement.

BP 6.3 Mon 15:30 BAR 0106

Magnetic fields help magnetotactic bacteria navigate complex environments — Agnese Codutti[1,2], Mohammad Charsooghi[1], Konrad Marx[3], Elisa Cerda-Donate[1], Omar Munoz[3], Paul Zaslansky[1], Vitali Telezki[3], Tom Robinson[1], Damien Faivre[1,4], and •Stefan Klumpp[3] — [1]MPI of Colloids and Interfaces, Potsdam — [2]TU Munich — [3]University of Göttingen — [4]Aix-Marseille Université, CEA, CNRS, BIAM, Saint Paul lez Durance, France

To study swimming of magnetotactic bacteria in a near-realistic sediment environment resembling those in their natural habitat, we produced microfluidic channels that contained sediment-mimicking obstacles. These obstacle channels were produced based on microCT reconstructions of sediment samples. We characterized the swimming of magnetotactic bacteria through these channels and found that swimming throughput was highest for intermediate magnetic fields. This observation was confirmed by extensive computer simulations using an active Brownian particle model, parameterized based on experimental trajectories. The simulations indicate that swimming at strong field is impeded by the trapping of bacteria in corners that require transient swimming against the magnetic field for escape. At weak fields, the direction of swimming is almost random, making the process inefficient as well. We confirmed the trapping effect in our experiments and showed that lowering the field strength allows the bacteria to escape.

BP 6.4 Mon 15:45 BAR 0106

Mechanical strain sensing and growth of rod-shaped Escherichia coli independent of cell wall synthesis — •Lars Renner[1], Felix Wong[2], Ariel Amir[2], Yuki Kitahara[3], and Sven van Teeffelen[3] — [1]Leibniz Institute of Polymer Research, Dresden — [2]Harvard University, Cambridge, USA — [3]Universite de Montreal, Canada

One of the central questions in bacterial cell biology is how specific shapes evolved and are maintained. It is remarkable how bacteria can precisely control the cellular processes regulating cell shape. However, many of the underlying biophysical cues are largely unknown. We set out to understand how mechanical stress affects rod-shape maintenance. Specifically, we combine microfabrication tools and mathematical modelling to identify a stress-based mechanism that regulates shape in rods. We then examined the influence of the biomolecular machinery that builds the cell wall and found that rod-shaped cells retain the ability to expand their envelopes differentially in response to locally varying mechanical forces. Thus, cell-wall cleaving enzymes appear to represent an alternative pathway for coupling cell envelope growth to mechanical forces that is distinct from cell wall insertion.

15 min. break

Invited Talk BP 6.5 Mon 16:15 BAR 0106

Mechanical and electrical properties of bacterial biofilms modulate antibiotic tolerance — •Berenike Maier — Institute for Biological Physics and Center for Molecular Medicine Cologne, University of Cologne

Aggregation into colonies and biofilms can enhance bacterial survivability under antibiotic treatment. Yet, the transition between the life as an individual cell and life within a biofilm is poorly understood. We investigate this transition using the human pathogen *Neisseria gonorrhoeae* (gonococcus). Within minutes, these bacteria self-assemble into spherical colonies comprising thousands of cells. We show that freshly assembled colonies are reminiscent of liquid droplets whose viscosity can be tuned by the pilus-mediated attractive force between bacterial cells. The viscosity correlates with antibiotic tolerance. Next to mechanical properties, we investigate the electrical properties of gonococcal colonies. We show that once the colonies have reached a critical size, the membrane polarization transitions from uncorrelated to collective dynamics. The spatial polarization pattern correlates with patterns of distict growth rates and antibiotic tolerance. In summary, both mechanical and electrical properties of bacterial colonies affect survivability under external stresses.

BP 6.6 Mon 16:45 BAR 0106

Acclimatization of filamentous cyanobacteria to light and pH - from individual to colony-scale — •Franziska Papenfuss, Sarah Haeger, Maximilian Kurjahn, Antaran Deka, and Stefan Karpitschka — MPI for Dynamics and Self-Organization, Göttingen, Germany

Photoautotrophic cyanobacteria contribute about 10 % to the net pri-

mary production of earth's biosphere. Acclimatization to fluctuating environmental conditions supported their sustained existence over a few billion years, but the underlying mechanisms remain elusive. Here, we investigate three species of filamentous cyanobacteria, cultivated for three weeks at different light-intensities (0.25-8 μE) and pH buffered to specific values between 6.8-8.4 or unbuffered. During cultivation, micro-scale parameters like the abundance of photopigments and the velocity of single filaments as well as macro-scale parameters like growth rate, pH and colony morphology were tracked. In unbuffered cultures, pH varies between 6.5-10, depending on light driven photosynthesis. Filaments start to aggregate at high densities but mainly independent of illumination and pH. Neither is the growth rate influenced by pH, however it is positively correlated to illumination. Nevertheless, in some species, pH seems to influence the filament gliding velocity and photopigmentation. Thus, our investigations show that pH is not only a consequence of the photosynthetic activity, but also influences the acclimatization of the cyanobacteria in a regulating feedback mechanism.

BP 6.7 Mon 17:00 BAR 0106

Molecular Dynamics Simulation of the Polymer Layering on the Surface Layer Proteins of Methanosarcina acetivorans — •Jonathan Hungerland[1], Aitolkyn S. Uali[2], Po-Heng Lee[3], and Ilia A. Solov'yov[1] — [1]Dept of Physics, University of Oldenburg — [2]Dept of Chemistry, Gumilyov Eurasian National University — [3]Dept of Civil and Environmental Engineering, Imperial College London

The archaea of the type Methanosarcina can produce Methane in an efficient, anaerobic, symbiotic process with Geobacter metallireducens. Their symbiosis is a so-called direct interspecies electron transfer (DIET), which is not limited by diffusion and has potential application in prospective energetically net-positive, anaerobic waste-water treatment. However, the mechanisms underlying DIET are yet unclear. The Methanosarcina species that coat themselves in layers of Methanochondroitin polymers were found to be capable of DIET. Therefore, the polymers might be crucial for the DIET of Methanosarcina species. The performed molecular dynamics simulations generate an atomistic picture of the Methanochondroitin layers accounting for the porous surface layer proteins aiming to suggest potential charge-transfer mechanisms into the cell and might reveal the role of the surface layer pores.

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

Time: Monday 15:00–18:15 Location: ZEU 160

BP 7.1 Mon 15:00 ZEU 160

Chiral motion of actively driven objects in discrete steps towards a remote target — •Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

We address the motion of chiral actively driven objects that move in discrete steps on a flat substrate [1]. While closed polygon-shaped trajectories are found in the case of unperturbed motion, the dynamics becomes surprisingly rich and nonlinear, if the objects additionally head for a fixed remote target. In that situation, cycloidal-like, straight, zigzag-type, doubled zigzag, quadrupled zigzag, and further period-doubled types of trajectory emerge, besides chaotic behavior. Additionally, we investigate the motion of crowds of such objects under explicit mutual alignment interaction. In the absence of fluctuations, collective orientational ordering occurs also in the chaotic regime, in combination with spatial gathering of the particles. Conversely, fluctuations and polydispersity in target alignment counteract orientational ordering. Our results may apply to various types of actively driven objects, for instance, light-responsive bacteria, laser-controlled colloidal particles, or hoppers on vibrated substrates.

[1] A. M. Menzel, resubmitted.

BP 7.2 Mon 15:15 ZEU 160

Polar flocks with discretized directions: the active clock model approaching the Vicsek model — •Matthieu Mangeat, Swarnajit Chatterjee, and Heiko Rieger — Universität des Saarlandes, Saarbrücken, Germany

We study the off-lattice two-dimensional q-state active clock model (ACM) [EPL **138**, 41001 (2022)] as a natural discretization of the Vicsek model (VM) [PRL **75**, 1226 (1995)] describing flocking. The ACM consists of particles able to move in the plane in a discrete set of q equidistant angular directions, as in the active Potts model (APM) [EPL **130**, 66001 (2020); PRE **102**, 042601 (2020)], with a local alignment interaction inspired by the ferromagnetic equilibrium clock model. A collective motion emerges at high densities and low noise. We compute phase diagrams of the ACM and explore the flocking dynamics in the region, in which the high-density (polar liquid) phase coexists with the low-density (gas) phase. We find that for a small number of directions, the flocking transition of the ACM has the same phenomenology as the APM, including macrophase separation and reorientation transition from transversal to longitudinal band motion as a function of the particle self-propulsion velocity. For a larger number of directions, the flocking transition in the ACM becomes equivalent to the one of the VM and displays microphase separation and only transverse bands, i.e. no reorientation transition. Concomitantly also the transition of the $q \to \infty$ limit of the ACM, the active XY model, is in the same universality class as the VM. We also construct a coarse-grained hydrodynamic description akin to the VM.

BP 7.3 Mon 15:30 ZEU 160

Tracer-induced temperature difference in motility-induced phase separation — •Lukas Hecht, Iris Dong, and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstr. 8, D-64289 Darmstadt, Germany

Previous studies of overdamped active Brownian particles (ABPs) mixed with passive tracers have shown that self-propulsion can induce motility-induced phase separation (MIPS) for large enough particle density and self-propulsion speed [1]. Here, we present our study on overdamped ABPs mixed with inertial passive tracers. We show that MIPS features different kinetic temperatures in the dense and the dilute phase if the passive tracers are sufficiently heavy (inertial). Remarkably, unlike for underdamped ABPs [2,3], neither the overdamped ABPs nor the passive tracers alone would feature such a temperature difference in coexisting phases. The observed temperature difference is accompanied by a violation of the equipartition theorem and strongly depends on the self-propulsion speed and the particle density. This allows us to tune the temperature difference from a cold dense and hot dilute phase to the counterintuitive opposite case in which the dense phase is hotter than the dilute phase. These findings open a route to create active materials with a persistent temperature profile by inserting active particles and tuning their self-propulsion speed accordingly.

[1] J. Stenhammar et al., Phys. Rev. Lett. 114, 018301 (2015).
[2] S. Mandal et al., Phys. Rev. Lett. 123, 228001 (2019).
[3] L. Hecht et al., Phys. Rev. Lett. 129, 178001 (2022).

BP 7.4 Mon 15:45 ZEU 160

Collective motion in two-dimensional colloidal systems with effective (active) self-propulsion due to time-delayed feedback — •Robin A. Kopp and Sabine H. L. Klapp — ITP, TU Berlin, Berlin, Germany

In recent years, delayed feedback in colloidal systems has become an active and promising field of study [1,2], key topics being history dependence and the manipulation of transport properties. Here we study the dynamics of a two-dimensional colloidal suspension, subject to time-delayed feedback, where time-delayed feedback can be interpreted as a mechanism of effective self-propulsion, i.e., activity [3]. To this end we perform overdamped Brownian dynamics simulations, where the particles interact through a Weeks-Chandler-Andersen potential. Furthermore, each particle is subject to a Gaussian, repulsive feedback potential, that depends on the difference of the particle position at the current time, and at an earlier time. We observe and quantitatively study the emergence of dynamical clustering and collective motion characterized by a nonzero mean velocity and provide a possible explanation for the underlying mechanism combining single-particle and mean-field-like effects.

[1] S. A. M. Loos, and S. H. L. Klapp, Scientific Reports **9**, 2491 (2019)

[2] M. A. Fernandez-Rodriguez et al., Nature Communications **11**, 4223 (2020)
[3] R. A. Kopp and S. H. L. Klapp, arXiv:2210.03182 (2022)

BP 7.5 Mon 16:00 ZEU 160

Inverted Sedimentation of Active Particles in Unbiased ac Fields — •José Carlos Ureña Marcos and Benno Liebchen — Institut für Physik Kondensierter Materie, TU Darmstadt, Darmstadt, Germany

Biological microswimmers can steer autonomously and use this ability to perform sophisticated tasks. Synthetic microswimmers do not yet reach the same degree of autonomy, and need to be controlled externally if they are to carry out tasks such as targeted cargo delivery or microsurgery. While much progress has been made recently to control their motion based on external forces or gradients, e.g. in light intensity, which have a well-defined direction or bias, little is known about how to steer APs in situations where no permanent bias can be realized.

Here, we show that ac fields with a vanishing time average provide an alternative route to steering APs. We exemplify this route for inertial APs in a gravitational field, observing that a substantial fraction of them persistently travels in the upward direction upon switching on the ac field, resulting in an inverted sedimentation profile at the top wall of a confining container. Our results offer a generic control principle which could be used in the future to steer active motion, to direct collective behaviors and to purify mixtures.

15 min. break

Invited Talk BP 7.6 Mon 16:30 ZEU 160

Long-range communications enable the hierarchical self-organization of active matter — •Igor Aronson[1], Alexander Ziepke[2], Ivan Maryshev[2], and Erwin Frey[2] — [1]Pennsylvania State University, USA — [2]Ludwig-Maximilians-University, Munich, Germany

The most distinct markers of life are the ability to move (locomotion), consume energy (metabolism), process information, and form multi-cellular aggregates. Many biological systems exhibit long-range signaling strategies for evolutionary advantage. We explore the multiscale self-organization of interacting self-propelled agents that locally process information transmitted by chemical signals. The communication capacity dramatically expands their ability to form complex structures, allowing them to self-organize through a series of collective dynamical states at multiple hierarchical levels.

The consequent study shows that information exchange by acoustic waves between the self-propelled units creates a slew of multifunctional structures. Each unit is equipped with an acoustic emitter and a detector in this realization. The swarmers respond to the resulting acoustic field by adjusting their emission frequency and migrating toward the strongest signal. We find self-organized structures with different morphology, including snake-like self-propelled entities, localized aggregates, and spinning vortices. Our results provide insights into the design principles of communicating active particles capable of performing complex tasks.

BP 7.7 Mon 17:00 ZEU 160

Arrested by heating — •Corinna C. Maass[1,2], Prashanth Ramesh[2,1], and Maziyar Jalaal[3] — [1]University of Twente, Enschede, Netherlands — [2]MPI for Dynamics and Self-organization, Göttingen, Germany — [3]Universiteit van Amsterdam, Amsterdam, Netherlands

Active droplets are a class of microswimmers driven by chemical reactions at the droplet interface. Typically, the activity is powered by an advection-diffusion instability in the chemohydrodynamic fields around the droplet that is characterised by the Péclet number Pe of chemical transport. With increasing Pe, higher hydrodynamic modes at the interface cause the droplet to transition from inactivity, to steady, to reorienting, to fully unsteady motion. Here, we demonstrate that it is possible to change Pe reversibly and in situ by thermally activated changes in the chemical enviroment, and thereby to control the motility of the droplet.

BP 7.8 Mon 17:15 ZEU 160

Chiral active particles with non-reciprocal couplings: results from particle-based simulations — •Kim L. Kreienkamp and Sabine H. L. Klapp — Technische Universität Berlin, Germany

Non-reciprocal interactions manifest their drastic impact on the collective dynamics of active matter systems by changing, for example, the general type of observed instabilities [1] and leading to time-dependent states [2,3]. In particular, the combination of non-reciprocity and chirality in terms of intrinsically rotating chiral active particles ("circle swimmers") reveals intriguing non-trivial time-dependent collective dynamics [1].

After having developed an understanding of the collective dynamics on the continuum level in previous work [1], we here present first results of particle-based simulations of chiral active particle systems with non-reciprocal alignment couplings. Indeed, quantitative predictions from continuum approaches are somewhat limited by the approximations made during the coarse-graining process. Thus, the first goal of our particle-based simulations is to explore the validity of the previously obtained continuum results regarding the overall state diagram. Second, we aim at investigating microscopic aspects of the various time-dependent states. Finally, we discuss possibilities to characterize the thermodynamic behavior of the non-reciprocal chiral system based on the stochastic trajectories obtained in particle-resolved simulations.

[1] K. L. Kreienkamp and S. H. L. Klapp, New J. Phys. (2022).
[2] M. Fruchart et al., Nature 592, 363 (2021).
[3] Z. You et al., PNAS 117, 19767 (2020).

BP 7.9 Mon 17:30 ZEU 160

Lattice-induced freezing in active systems unveils dynamic crystallites with square ordering — •Aritra K. Mukhopadhyay[1], Peter Schmelcher[2,3], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, 64289 Darmstadt, Germany. — [2]Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany. — [3]The Hamburg Centre for Ultrafast Imaging, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany.

Active matter, comprising self-propelled particles like bacteria, colloidal microswimmers, or granular microflyers is currently attracting enormous attention for its ability to self-organize into complex nonequilibrium structures. In this work, we report on a new state of dynamic active crystallites, which occurs when exposing active particles to a spatially periodic potential. These crystallites require activity to emerge, adopt the structure of the underlying lattice (e.g. square rather than hexagonal close packing), and are continuously in motion. This new phase unifies the structural properties of crystals with the dynamical properties of disordered fluids. Our work thus unveils a route to creating a new state of active materials with an intrinsic structure that can be externally controlled.

BP 7.10 Mon 17:45 ZEU 160

Shape-dependent collective motion: cohesive groups and cargo transport of colloidal rods — Philipp Stengele, •Anton Lüders, and Peter Nielaba — Universität Konstanz, Konstanz, Deutschland

In active toy model systems where colloids interact via predefined social interaction rules as well as steric collisions, the shape of the individual particles strongly influences emerging collective behavior. We study this based on two example systems using Brownian dynamics simulations (without hydrodynamic interactions). Firstly, we investigate a simple perception model in which colloidal rods move actively if predefined visual stimuli exceed a certain threshold. Here, we find an aspect ratio range where the rods form a dilute cohesive group with a time-independent particle distribution. If the aspect ratio surpasses this range, the rods slowly drift apart. Secondly, we look into the cargo capture and transport of a passive rod using a dense swarm of active spheres which form a hexagonal cage with a cavity for the cargo. Again, the aspect ratio of the rod proves to be crucial, as we find geometric restrictions that must be met to stabilize the cavity. Our work underlines that the shape (here, the aspect ratio) of the particles in active matter systems must be carefully considered while defining interaction rules to perform specific tasks.

BP 7.11 Mon 18:00 ZEU 160

Active Chiral Nematics — •Rüdiger Kürsten[1,2,3] and Demian Levis[1,2] — [1]Departament de Física de la Matèria Condensada, Universitat de Barcelona, Barcelona, Spain — [2]Universitat de Barcelona Institute of Complex Systems (UBICS), Barcelona, Spain — [3]Institut für Physik, Universität Greifswald, Greifswald, Germany

We study inherently chiral self-propelled particles in two dimensions that are subjected to nematic alignment interactions and rotational noise. By means of both, homogeneous and spatially resolved mean

field theory we identify various different flocking states. We confirm the presence of the predicted phases using agent-based simulations. We emphasize that special care has to be taken within the simulations in order to avoid artifacts. We present a non-standard simulation technique in order to avoid those artifacts.

BP 8: Cell Mechanics I

Time: Tuesday 9:30–13:00 Location: BAR Schö

BP 8.1 Tue 9:30 BAR Schö

Chiral flows can drive pattern formation in viscoelastic surfaces — •Eloy de Kinkelder[1,2], Elisabeth Fischer-Friedrich[3,4], and Sebastian Aland[1,2] — [1]TU Bergakademie Freiberg, Freiberg, Germany — [2]HTW Dresden, Dresden, Germany — [3]TU Dresden, Dresden, Germany — [4]BIOTEC, Dresden, Germany

During division in animal cells, the actomyosin cortex has been found to exhibit counter-rotating cortical flows along the axis of division. These are also known as chiral flows. Notably, the chiral flows were shown to influence cellular rearrangements and drive the left-right symmetry breaking in developing organisms. At the current state, no numerical simulations have been done to study the influence of chiral flows on the cell cortex shape. To deepen the insight on that matter, we present here a numerical study of an axi-symmetric viscoelastic surface embedded in a viscous fluid. On this surface we impose a generic counter rotating force field to investigate its influence on the surface shape and material transport. Notably, we find that a large areal relaxation time results in flows towards the equator of the surface. These flows assist the transport of a surface concentration during the forming of a contractile ring. Accordingly, we show that chiral forces by themselves can drive pattern formation and stabilise contractile rings at the equator.

BP 8.2 Tue 9:45 BAR Schö

Neutrophil mechanotransduction during durotaxis — •Fatemeh Abbasi[1], Matthias Brandt[2], and Timo Betz[1] — [1]Third Institute of Physics,Biophysics, Georg August University Göttingen — [2]Institute of Cell Biology, ZMBE, University of Münster

In Vivo, cells experience complex tissue environments with various chemical and physical features. 3D confinement is one of the major physical obstacles for cells in their natural environment. Neutrophils are among the most abundant immune cells in our body, which have to cope with various physical constrictions on their way from production to the infection site. In addition to confinement, the stiffness of the microenvironment is another mechanical feature these rapidly moving cells are exposed to. Neutrophils experience various tissue stiffness, from 1 kPa (bone marrow) to 20 MPa (bone). Previous studies have demonstrated that these cells are responsive to their microenvironment stiffness by adjusting their adhesion and spreading. Based on this knowledge we decided to combine confinement and stiffness change and investigate the impact of 3D stiffness gradient on cell behaviour and migration, a fact called durotaxis. We hypothesized that stiffness gradient might be a triggering factor of neutrophil migration toward the infection site. We confine neutrophils in between 2 layers of polyacrylamide hydrogels with 2 different stiffness and keep this distance stable for the desired period of time to investigate cell mechanotransduction during durotaxis from different points of view. Our preliminary results regarding the neutrophil durotaxis show a surprising and transient force peak on the soft substrate during cell shifting.

BP 8.3 Tue 10:00 BAR Schö

Red blood cell lingering modulates hematocrit distribution in the microcirculation — •Yazdan Rashidi[1], Greta Simionato[2], Qi Zhou[3], Thomas John[1], Alexander Kihm[1], Mohammed Bendaoud[1], Timm Krueger[3], Miguel o. Bernabeu[3], Lars Kaestner[1], Mattias w. Laschke[2], Michael d. Menger[2], Christian Wagner[1], and Alexis Darras[1] — [1]Experimental Physics, Saarland University, 66123 Saarbruecken, Germany — [2]Institute for Clinical and Experimental Surgery, Saarland University, 66421 Homburg, Germany — [3]School of Engineering, University of Edinburgh, Edinburgh EH9 3FD, United Kingdom

The distribution of red blood cells (RBCs) in the microcirculation determines how oxygen is delivered to tissues and organs. This process relies on the partitioning of RBCs at successive microvascular bifurcations. It is known that RBCs partition disproportionately to the blood flow rate, therefore leading to heterogeneity of the hematocrit in microvessels. Usually, downstream of a bifurcation, the vessel branch with a higher fraction of blood flow receives a higher fraction of RBC flux.

However, deviations from this phase-separation law have been observed in recent works. Here, we quantify how the microscopic behavior of RBCs lingering influences their partitioning, through combined in vivo experiments and in silico simulations. We quantify the cell lingering at capillary-level bifurcations and demonstrate that it correlates with deviations from the phase-separation process from established empirical predictions by Pries et al.

BP 8.4 Tue 10:15 BAR Schö

Mechanical fingerprint of the intra-cellular space — •Till M. Muenker, Bart E. Vos, and Timo Betz — University of Göttingen, Göttingen, Germany

Many important cellular functions such as organelle positioning and internal cargo transport are dependent on the viscoelastic intracellular mechanical properties of cells. A range of different mechanical models has been proposed to describe these properties. Whilst simple models such as Maxwell or Kelvin-Voigt models don't seem sufficient to capture the full complexity of cells, more elaborate models like generalized Kelvin-Voigt models require a huge number of parameters. This hinders the comparison and interpretation of experimental findings. Further, from a physics perspective, cells are systems out of thermodynamic equilibrium, permanently consuming metabolic energy to carry out mechanical work. The level of "non-equilibrium" can be proposed as an indicator for cell type, cell state or even diseases. To determine both, the viscoelastic properties and the cellular activity, we use optical tweezers based active and passive microrheology in a diverse group of 9 different cell-types. Surprisingly, despite differences in origin and function, the complex moduli of all cell types can be described using a 4 parameter based fractional Kelvin-Voigt model. Additionally, the frequency dependent activity can be described with a simple power law. This approach allows to reduce those complex and frequency dependent properties down to a fingerprint of 6 parameter. Further principal component analysis shows that only 2 of them may be sufficient to characterize the mechanical intracellular state.

15 min. break

Invited Talk BP 8.5 Tue 10:45 BAR Schö

Microtubule Lattice Dynamics — Subham Biswas[1], Rahul Grover[2], Cordula Reuther[2], Mona Grünewald[1], Stefan Diez[2], and •Laura Schaedel[1] — [1]Saarland University, Saarbrücken, Germany — [2]TU Dresden, Germany

Microtubules are dynamic cytoskeletal filaments that grow and shrink by subunit addition or removal at their tips. In contrast, the microtubule lattice far from the tips was long considered to be static. The discovery of subunit loss and incorporation along the lattice far from the tips - termed lattice dynamics - led to a paradigm shift and revealed a new dimension of microtubule dynamics.

Microtubule lattice dynamics occur in vitro as well as in living cells and contribute to microtubule organization and resilience to mechanical stress. Yet, it is largely unknown which cellular mechanisms are involved in their regulation. Recent discoveries suggest that microtubule-associated proteins (MAPs), which control a variety of properties of intracellular microtubules, are a key factor in the regulation of lattice dynamics. Here, we take a closer look at MAP-regulated microtubule lattice dynamics.

BP 8.6 Tue 11:15 BAR Schö

Force generation in human blood platelets by filamentous actomyosin structures — •Anna Zelena[1], Johannes Blumberg[2], Ulrich S. Schwarz[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, Georg-August-University of Göttingen, Germany — [2]Institute for Theoretical Physics, University of Heidelberg, Germany

Blood platelets are central elements of the blood clotting response after wounding. Upon vessel damage, they adhere to the surrounding matrix of the vessel and contract the emerging blood clot, thus helping to restore normal blood flow. The blood clotting function of platelets has been shown to be directly connected to their mechanics and cytoskeletal organization. The reorganization of the platelet cytoskeleton during spreading occurs within minutes and leads to the formation of contractile actomyosin bundles, but it is not known how this structure formation corresponds to force generation. In this study, we combine fluorescence imaging of the actin structures with traction force measurements in a time-resolved manner. We find that force generation is localized in few hotspots, which spatially align very closely with the visualized end points of the fibrous actin structures and do not change much with time. Moreover we show that force generation is a very robust mechanism independent of changes in the amount of added thrombin in solution or fibrinogen coverage on the substrate, suggesting that force generation after platelet activation is a threshold phenomenon that ensures reliable blood clot contraction in diverse environments.

BP 8.7 Tue 11:30 BAR Schö

How to build muscle? Sarcomeric pattern formation by non-local interactions — •Francine Kolley[1,2], Clara Sidor[3], Frank Schnorrer[3], and Benjamin M. Friedrich[1,2] — [1]Physics of Life, TU Dresden — [2]cfaed, TU Dresden — [3]IBDM,Aix Marseille University

Striated muscles drive all voluntary movements and are highly organized in crystal-like structures, comprising different filament types on a micrometer scale. The specific size of a sarcomere is set by the giant protein titin. Titin links the molecular motor myosin in the middle of a sarcomere to the so-called Z-disc, which is rich in actin crosslinkers at the sarcomere boundary. Despite the importance of the repeated structures of theses sarcomeres for muscle functionality, it is poorly understood how they self-assemble during muscles development.To investigate this question, we introduce theoretical models based on putative mechanism. We can show with a minimal Mean-field model that a non-local interaction between the key proteins is sufficient for the emergence of periodic patterns. Agent-based simulations of this model reveal the influence of small-number fluctuations. We can expand this model to include additional properties, such as different myosin bindings or the catch-bond behavior of the Z-disc crosslinker α-actinin. In addition, from analyzing images of the *Drosophila* flight muscles during early developmental stages, provided by Schnorrer Lab, we are able to identify α-actinin and titin as the first proteins forming periodic patterns with myosin, while actin follows later, constraining possible models.

15 min. break

BP 8.8 Tue 12:00 BAR Schö

Impact of oxidative stress on the mechanical properties of isolated mitochondria — •Yesaswini Komaragiri[1,2], Muzaffar H Panhwar[1,2], Bob Fregin[1,2], Gayatri Jagirdar[3], Carmen Wolke[3], Stefanie Spiegler[1,2], and Oliver Otto[1,2] — [1]Institut für Physik, Universität Greifswald, Friedrich-Ludwig-Jahn-Str. 15a, 17489 Greifswald, Germany — [2]DZHK, Greifswald, Universitätsmedizin Greifswald, Fleischmannstr. 42, 17489 Greifswald, Germany — [3]Universitätsmedizin Greifswald, Ferdinand-Sauerbruch-Strasse, 17475 Greifswald, Germany

Mitochondria are essential in various physiological processes, including the homeostasis of reactive oxygen species (ROS) as key intracellular signaling molecules. While it is already established that mechanical properties are a crucial parameter in characterizing and comprehending biological systems such as cells and tissues, little is known about the significance of organelle mechanics for cell function. Here, we demonstrate the application of real-time fluorescence and deformability cytometry for the label-free and high-throughput analysis of mitochondria isolated from C6 glial cells. Our data on several thousands of viable mitochondria indicate that their deformation is shear stress dependent. We studied the effect of exogenously and endogenously generated ROS on mitochondria mechanics in two proof-of-concept studies. Under both conditions, we observed a decrease in size while the deformation increased relative to a control condition. The results suggest a general biophysical mechanism of how mitochondria respond to oxidative stress.

BP 8.9 Tue 12:15 BAR Schö

New applications for the direct method in 3D traction force microscopy — •Johannes Blumberg[1,2], Simon Brauburger[1,2], and Ulrich Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University — [2]Bioquant, Heidelberg University

Traction force microscopy (TFM) estimates the mechanical forces of cells adhering to an elastic substrate by measuring by the movement of embedded marker beads. It has become a standard tool to study the mechanobiology of single cells or cell monolayers on flat two-dimensional (2D) substrates, but three-dimensional (3D) setups provide new challenges. Although the inverse method of force inference by minimization of a loss function has become the standard method for 2D TFM, for 3D TFM the direct method of directly calculating stress and surface traction from strain becomes an attractive alternative, for example when performing 3D TFM with elastic beads in organisms, tumor spheroids or organoids. We explain how this method works in practice and how it compares to the inverse method.

BP 8.10 Tue 12:30 BAR Schö

Profilin Regulating the Polymerisation Velocity of Actin — •Lina Heydenreich and Jan Kierfeld — TU Dortmund University, 44227 Dortmund, Germany

F-Actin, as a part of the cytoskeleton, drives crucial biological processes like cell motility, where the control of the polymerisation speed is essential. Experiments in [1] show a maximal polymerisation speed of F-actin at high concentrations of profilin and actin.

We present a kinetic model of F-actin growth in the presence of profilin and obtain an exact result for the mean growth velocity which is in agreement with stochastic simulations, and explains the experimental data. The maximal growth speed is limited by the release rate of profilin from filamentous actin. In the limit where nearly all actin monomers are bound to profilin, the polymerisation speed follows the Michaelis-Menten kinetics.

By analysing the presented model, we can examine the influence of an external force and the influence of profilin on the fluctuations and precision of the polymerisation. Additionally we can give constraints on the concentrations to obtain a saturation of the growth velocity.

[1] Johanna Funk et al. "Profilin and formin constitute a pacemaker system for robust actin filament growth". eLife 8 (2019), e50963

BP 8.11 Tue 12:45 BAR Schö

Development of a platform for accessing the membrane tension of cells in microchannels — •Eric Sündermann, Bob Fregin, Doreen Biedenweg, Stefanie Spiegler, and Oliver Otto — ZIK HIKE, University of Greifswald, Greifswald, Germany

The development of high-throughput methods for cell mechanical research is becoming increasingly important in biology, medicine and physics as the analysis of large samples opens up possibilities for basic science and clinical use. Currently, various techniques are available, but hardly any can discriminate between membrane and bulk contributions to the mechanical properties of a cell.

Here, we combined deformability cytometry with fluorescence lifetime imaging microscopy (FLIM) to study the response of membrane tension to hydrodynamic stress. Myeloid precursor cells were first stained with Flipper-TR®, a fluorescent dye with a lifetime proportional to the membrane tension, and then flushed through the constriction of a microfluidic chip, where they deform under a shear stress. Under steady-state conditions, our data shows that the membrane tension of cells increases with increasing hydrodynamic stress, as expected. Exposing cells to methyl-ß-cyclodextrin to reduce the amount of cholesterol in the cell membrane leads to a reduction in membrane tension while the bulk Young's modulus is not affected.

These results highlight the potential of microfluidic technologies to quantify the contribution of different cell components to its overall mechanical phenotype.

BP 9: Active Matter III (joint session BP/CPP/DY)

Time: Tuesday 9:30–12:30 Location: TOE 317

BP 9.1 Tue 9:30 TOE 317

Gliding motility and reorientation of flagellated microbes on curved surfaces — •Alexandros Fragkopoulos[1], Nicolas Fares[1,2], and Oliver Bäumchen[1] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]University of Bordeaux, CNRS, LOMA, UMR 5798, 33400 Talence, France

The model organism *Chlamydomonas reinhardtii*, a unicellular biflagellated microalga, can adhere and colonize almost any surface under particular light conditions. Once the cells attach to a surface, an intraflagellar transport machinery translocates the cell body along the flagella, which are oriented in a 180° configuration. This motion is known as gliding motility. Even though the cells firmly adhere to surfaces, they are able to reorient through different physical mechanisms [1]. With the use of the orientation autocorrelation function, we find that cells exhibit large reorientation events shortly after their initial attachment to a surface, while at longer time scales they are primarily constrained to 1D motion. On cylindrical surfaces, the large reoriations cause the cells to predominantely align in the direction of the minimum principle curvature. We quantify the curvature-induced alignment using the nematic order parameter and reveal that the minimum surface curvature required for cell alignment is comparable to the static flagella curvature.

[1] S. Till, et al., *Phys. Rev. Res.*, (Accepted)

BP 9.2 Tue 9:45 TOE 317

Efficiency of navigation strategies for active particles — •Lorenzo Piro[1], Ramin Golestanian[1,2], and Benoit Mahault[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, United Kingdom

Optimal navigation in complex environments is a problem with multiple applications ranging from designing efficient search strategies to engineering microscopic cargo delivery. When motion happens in presence of strong external forces, route optimization is particularly important as active particles may encounter trapping regions that would substantially slow down their progress.

Here, considering a self-propelled agent moving at a constant speed, we study the efficiency of Zermelo's classical solution. Investigating both cases of motion on the plane and on curved surfaces, we focus on the regime where the external force exceeds self-propulsion in finite regions. There, we show that, despite the fact that most trajectories following the trivial policy of going straight get arrested, the Zermelo policy allows for a comprehensive exploration of the environment.

However, our results also indicate an increased sensitivity of the Zermelo strategy to initial conditions, which limits its robustness and long-time efficiency, particularly in presence of fluctuations. These results suggest an interesting trade-off between exploration efficiency and stability for the design of control strategies to be implemented in real systems.

BP 9.3 Tue 10:00 TOE 317

Run with the Brownian Hare, Hunt with the Deterministic Hounds — •Davide Bernardi[1] and Benjamin Lindner[2,3] — [1]Italian Institute of Technology, Ferrara, Italy — [2]Bernstein Center for Computational Neuroscience, Berlin, Germany — [3]Institut für Physik, Humboldt-Universität zu Berlin

Pursuit and evasion are vital to most animal species and play an important role in many human activities. Traditionally, chase-and-escape models have been studied in the framework of game theory, or in detailed models that can be studied only through numerical simulations and that lack generalization power.

Here, we present analytic results for the mean time and energy used by a pack of deterministic hounds to capture a prey that undergoes Brownian diffusion. Depending on the number of chasers, we find that the mean capture time as a function of the prey's diffusion coefficient can be monotonically increasing, decreasing, or attain a minimum at a finite value. Furthermore, an optimal speed and number of chasing hounds exist, that depend on the baseline power consumption and drag coefficient of each chaser.

The present model can be seen as an analytically tractable basis for the theoretician's perspective on the growing field of smart microswimmers and autonomous robots.

BP 9.4 Tue 10:15 TOE 317

Function of Morphodynamics in Foraging *Physarum polycephalum* — •Lisa Schick[1], Mirna Kramar[2], and Karen Alim[1] — [1]School of Natural Sciences, Technical University of Munich, Germany — [2]Institute Curie, Paris, France

How network-forming fungi structure and reorganize their network morphology and thereby the carbon flows in the soil is key to understanding climate - yet hidden from us due to the long time scales of network dynamics and the soil itself. Here, the network-forming slime mold *Physarum polycephalum* serves as a model of network dynamics of a foraging network-forming life. We follow and quantify the network migration velocity and morphology of foraging *P. polycephalum*. We identify three distinct morphological states characterized by network compactness and density of moving fronts. Estimating the energetic cost of distinct states, we find that morphological variability allows the organism to balance the energetic costs of foraging and search strategy. Our observations allow us to project how resource availability might shift the balance and thereby affect network extension in foraging network-forming organisms.

BP 9.5 Tue 10:30 TOE 317

Unraveling the migratory behavior of a large single-celled organism — •Lucas Tröger, Florian Goirand, and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

Many cells face search problems, such as finding food, conspecifics, or shelter, and different search strategies can provide different chances for success. In contrast to most single-celled organisms the slime mold *Physarum polycephalum* forms a giant network-shaped cell while foraging for food. Which advantage does the giant cell at the verge to multicellularity provide? We experimentally investigate and quantify the long-time migratory behavior of small networks of *P. polycephalum* in the absence and in the presence of food, and develop a simple mechanistic model that successfully describes its migration. We find that *P. polycephalum* performs a run-and-tumble-like motion modified by self-avoidance to achieve superdiffusive migration. Furthermore, it tunes its short-time dynamics in order to adapt to environments with different amounts of available nutrients, while its long-time dynamics remain unchanged. This work shows how *P. polycephalum* controls the inherent stochasticity of its movement by simple rules, which may represent an evolutionary advantage.

15 min. break

BP 9.6 Tue 11:00 TOE 317

Controlling active turbulence by activity patterns — •Arghavan Partovifard, Josua Grawitter, and Holger Stark — Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Active fluids exhibit spontaneous and chaotic flow patterns which are known as active turbulence [1]. One of the current challenges in active matter is controlling and harnessing these flow patterns for powering processes at small scales [2]. As a simple realization of an active fluid, we consider a semi-dilute solution of active rods and study it within a numerical simulation of the governing equations that are formulated in terms of velocity and the orientational order tensor parameter fields.

We find that for a solution of pusher active rods there is a critical magnitude of activity above which the initially isotropic solution develops locally varying nematic order and turbulent-like fluid flow. Aiming to control the turbulent flow state, we pattern the activity with a square lattice of circular inactivity spots. We find that for a specific range of lattice parameters the flow field develops lanes of unidirectional flow with alternating directions while between them a row of corotating vortexes emerges; We call this state the laning state and it is multistable since different realizations of the random initial state of rods lead to different configurations of the laning state with various widths of the lanes. In this state, the director field develops nematic domains oriented toward the Leslie angle with respect to the flow.

[1] Wensink *et al.*, Proc. Natl. Acad. Sci. **109**, 14308-14313 (2012)
[2] Bowick *et al.*, Phys. Rev. X **12**, 010501 (2022)

BP 9.7 Tue 11:15 TOE 317

Active matter: From spontaneous to controlled phenomena.

— •Daniel Pearce — University of Geneva

Active matter is the study of materials able to move themselves. During this talk I will discuss how we can take advantage of the interplay between topological defects, geometry and topology to exercise control over active materials. By studying active nematic fluids on a curved surface, we can influence the position and orientation of topological defects according to their charge. This means specific nematic textures can be generated. By studying active contractile actomyosin gels, it is possible to show that only active topological defects with charge +1 can generate curvature, and the sign is related to the phase of the defect. This frees the process from the constraints of the Poincare-Hopf theorem and allows complex surfaces to be generated. This is demonstrated by recreating the shape of a freshwater hydra from the positions of the topological defects

BP 9.8 Tue 11:30 TOE 317

Nucleation of chemically active droplets — •Noah Ziethen and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Liquid-liquid phase separation emerged as a crucial organizing principle inside biological cells giving rise to a plethora of intracellular compartments. Unique to the cellular context, these condensates can consist of only a few hundred molecules and are affected by non-equilibrium processes. In particular, active chemical conversion between condensate material and proteins in the surrounding cytoplasm can control multiple aspects of the condensates. Yet, it is unclear how these reactions affect the spontaneous nucleation and dissolution associated with low particle numbers. Here, we investigate the influence of chemical reactions on the bistable region of active droplets using a stochastic field theory. We find an effective increase in the energy barrier and thus decelerated transitions between the homogeneous and the droplet state. Using classical nucleation theory, we approximate the full dynamics by diffusion in a free energy potential described by an analytical expression only depending on droplet radius and reaction rate. This analogy also allows us to determine the equivalence of the binodal line, so we can propose an extension of the equilibrium phase diagram to capture driven chemical reactions. Cells might use these effects to control the nucleation of intracellular droplets.

BP 9.9 Tue 11:45 TOE 317

Hydrodynamic description and transport coefficients in a model of active cellular aggregates — •Subhadip Chakraborti[1,2] and Vasily Zaburdaev[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

Complex multicellular aggregates consisting of a large number of interacting cells are ubiquitous in biology, ranging from bacterial biofilms to organoids, cell spheroids, and tumors. We consider colonies of *N. gonorrhoeae* bacteria as a prototypical example of cells that use retractile cell appendages to actively interact with a substrate and with each other. We construct a microscopic model on a 1D lattice taking into account the non-equilibrium bacterial motility driven by two crucial forces – cell-substrate and cell-cell interactions. We observe a phase transition from a homogeneous state to a clusterized state upon tuning the density and activity parameters. Using macroscopic fluctuation theory (MFT), we analytically derive hydrodynamics for the model system and calculate two density-dependent transport coefficients – the bulk-diffusion coefficient and the conductivity. The behavior of these transport coefficients successfully explains the non-equilibrium phase transition. We support our analytical findings with the results obtained numerically. Our theory provides a general framework for studying the non-equilibrium collective behavior of other dense cellular aggregates also, in the context of dynamics and their transport properties.

BP 9.10 Tue 12:00 TOE 317

Flocking of unfriendly species: The two-species Vicsek model — •Swarnajit Chatterjee[1], Matthieu Mangeat[1], Chul-Ung Woo[2], Heiko Rieger[1], and Jae Dong Noh[2] — [1]Saarland University, Saarbrücken, Germany — [2]University of Seoul, Seoul, Korea

We consider the two-species Vicsek model (TSVM) consisting of two kinds of self-propelled particles, A and B, that tend to align with particles from the same species and to anti-align with the other. The model shows a flocking transition that is reminiscent of the original Vicsek model [1]: it has a liquid-gas phase transition and displays micro-phase separation in the coexistence region where multiple dense liquid bands propagate in a gaseous background. The novel feature of the TSVM is the existence of two kinds of bands, one composed of mainly A-particles and one mainly of B- particles and the appearance of two dynamical states in the coexistence region: the PF (parallel flocking) state in which all bands of the two species propagate in the same direction, and the APF (anti-parallel flocking) state in which the bands of species A and species B move in opposite directions. When PF and APF states exist in the low-density part of the coexistence region they perform stochastic transitions from one to the other. The system size dependence of the transition frequency and dwell times shows a pronounced crossover that is determined by the ratio of the band width and the longitudinal system size. Our work paves the way for studying multispecies models with heterogeneous alignment interactions.

[1] T. Vicsek, A. Czirók, E. Ben-Jacob, I. Cohen, and O. Shochet, Phys. Rev. Lett. 75, 1226 (1995).

BP 9.11 Tue 12:15 TOE 317

Two-potential model for molecular motors — •Sophie Klempahn and Helmut Schiessel — Cluster of Excellence Physics of Life, Technical University of Dresden, Germany

Molecular motors are highly efficient biological machines, which drive systems away from equilibrium and realise key biological processes. For the description of the molecular motor action, discrete jump processes as well as energy barriers with height differences can be used. However, these models are based on symmetric conditions or unidirectional motion and therefore do not capture real biological systems with fuel gradients or where the motion is not unidirectional. To predict the effect of molecular motors on the density distribution of cargo particles in one dimension, we introduce a two potential model. This model represents the cargo particles as active particles, in which the binding of molecular motors to the cargo particle causes the active part of motion. Furthermore, we use two different energy landscapes for jumps to the left or right side, to include motors moving back- and forward, asymmetric environment or two different molecular motors acting on the same cargo particle in different directions. The solution of a master equation with different energy landscapes for jumps to the left and right side results in specific extremal points in the probability density of the cargo particles and shows a ratchet effect in case of periodic potentials.

BP 10: Evolution and Origin of Life

Time: Tuesday 9:30–12:15 Location: BAR 0106

Invited Talk BP 10.1 Tue 9:30 BAR 0106

Protein evolution in sequence landscapes: from data to models and back — •Martin Weigt — Sorbonne University, Paris, France

In the course of evolution, proteins diversify their sequences via mutations, while keeping their 3D structure and biological functions remarkably conserved. Modern sequence databases provide us with increasingly large samples for this sequence diversity. In my talk, I will describe how these samples can be used to infer data-driven protein sequence landscapes, using approaches borrowed from statistical physics or machine learning. In turn, we can model the interplay between mutation and selection in protein evolution as a stochastic process in these landscapes. I will illustrate these ideas in three examples: (i) the prediction of the effect of individual mutations in proteins, (ii) the modeling of experimental protein evoltuion, and (iii) the statistical design of artificial but functional proteins.

BP 10.2 Tue 10:00 BAR 0106

Non-equilibrium approaches to the origin of life — Thomas Matreux[1], Paula Aikkila[1], Corinna Kufner[2], Dominik Bucher[3], Almuth Schmid[1], Wolfgang Zinth[1], Dieter Braun[1], and •Christof Mast[1] — [1]LMU, Munich, Germany — [2]Harvard, Cambridge, USA — [3]TUM, Munich, Germany

Life is an out-of-equilibrium process, so its emergence must also have been decisively shaped and driven by the non-equilibrium systems present 4 billion years ago. We investigated how simple heat fluxes through geological networks of interconnected chambers created chemical niches from complex mixtures of prebiotically relevant substances, each with different prevailing concentration ratios. These "micro-labs" could thus enable a wide variety of prebiotic reactions and massively increase their yield and selectivity compared to bulk systems. We further measured the sequence selectivity of UV radiation on pseudogenomes built from subsets of codon sequences. Comparison with existing chronologies for codon and amino acid evolution suggests the importance of UV light as a selection pressure during the evolution of early life.

BP 10.3 Tue 10:15 BAR 0106

Unpredictable repeatability in evolutionary dynamics — •Suman Das and Joachim Krug — Institute for Biophysics, University of Cologne, Germany

Biological evolution proceeds through occurrence and fixation of mutations. But how repeatable are evolutionary trajectories? Is the evolution of specific well-adapted genotypes largely a matter of chance, or should we expect the same genotypes to evolve repeatedly? The answer depends in part on the probability distribution of mutational effect sizes. Repeatability is itself a random variable, and for light-tailed distributions it converges to its mean value in the limit of a large number of available mutations. However, for heavy-tailed distributions, we show that the repeatability is much higher but the distribution remains broad, and consequently the repeatability cannot be predicted based on the distribution. This non-self averaging effect is similar to those observed in certain disordered systems, and arises from the fact that the fixation process is dominated by a few mutations even in the limit of infinite mutation number. We discuss the behavior in various heavy-tailed regimes, and illustrate it with applications to empirical data on drug resistance evolution.

REF: S G Das and J Krug (2022). Unpredictable repeatability in molecular evolution. Proceedings of the National Academy of Sciences, 119(39):e2209373119.

BP 10.4 Tue 10:30 BAR 0106

Kinetics of Information Content in a Virtual Circular Genome — •Ludwig Burger, Tobias Thun, and Ulrich Gerland — Technical University of Munich

We study the kinetics of information content in an ensemble of oligonucleotides that undergo hybridization, dehybridization, non-enzymatic templated ligation and single-strand cleavage. The stability of hybridized complexes depends on the sequence because the dehybridization rate depends on the free hybridization energy. Mismatches are possible, but they lead to a thermodynamic and kinetic penalty. The information that is supposed to be "stored" in the ensemble is a circular genome as well as its complementary strand. Therefore, the oligonucleotides in the initial ensemble are chosen such that every element in the ensemble is part of the true genomic sequence. In most investigated scenarios, the initial ensemble loses its information content and no information amplification can be observed. Depending on the choice of ligation and cleavage rate, the loss of information can be driven by cleavage or ligation. Information loss by ligation is caused by templated ligation processes that produce long strands that do not resemble the true genomic sequence. This is the case if the hybridization site is too short or contains too many mismatches to guarantee correct alignment of template and ligated strands. Even though information amplification appears to be difficult to achieve, the timescale of information loss can be extended by tuning the hybridization energy or the concentration of short oligomers.

15 min. break

BP 10.5 Tue 11:00 BAR 0106

Evolutionary rescue of resistant mutants is governed by a balance between radial expansion and selection in compact populations — Serhii Aif[1,2], Nico Appold[1,2], Lucas Kampmann[3], Oskar Hallatschek[3,4], and •Jona Kayser[1,2] — [1]MPI für die Physik des Lichts, Erlangen, Germany — [2]MPZ für Physik und Medizin, Erlangen, Germany — [3]University of California, Berkeley, USA — [4]Leipzig University, Leipzig, Germany

Mutation-mediated treatment resistance is one of the primary challenges for modern antibiotic and anti-cancer therapy. Yet, how slower-growing resistant lineages may escape purifying selection via continued evolution is still unclear. Here, we introduce a system of fluorescence-coupled synthetic mutations to track the entire evolutionary trajectory of thousands of resistant lineages in expanding yeast colonies. We uncover that an underlying quasi-stable equilibrium between the opposing forces of radial expansion and natural selection, a phenomenon we term inflation-selection balance, enhances the evolutionary rescue of resistant lineages. Tailored computational models and agent-based simulations corroborate the fundamental nature of the observed effects and demonstrate the potential impact on drug resistance evolution in cancer. The described phenomena should be considered when predicting multi-step evolutionary dynamics in any mechanically compact cellular population, including pathogenic microbial biofilms and solid tumors. The insights gained will be especially valuable for the quantitative understanding of response to treatment, including emerging evolution-based therapy strategies.

BP 10.6 Tue 11:15 BAR 0106

Heat flows drive ionic and pH gradients — •Thomas Matreux[1], Almuth Schmid[1], Paula Aikkila[1], Kristian Le Vay[2], Johannes Raith[3], Bernhard Altaner[3], Bettina Scheu[4], Ulrich Gerland[3], Hannes Mutschler[2], Dieter Braun[1], and Christof B. Mast[1] — [1]Systems Biophysics, LMU Munich, Germany — [2]Biomimetic systems, TU Dortmund, Germany — [3]Physics of Complex Biosystems, TU Munich, Germany — [4]Earth and Environmental Sciences, LMU Munich, Germany

The first steps in the emergence of life on Earth occurred on rocks and their constituent phases with a feedstock of simple molecules. Our aim is to combine this background with physical non-equilibria such as thermal gradients, offering unique opportunities for molecular selection on all levels.

In this scenario, ions leached from mineral samples are selectively accumulated by heat flows through water-filled fractures. In contrast to up-concentration by dehydration or freezing, this actively alters the Magnesium:Sodium ratio to an extent that permits key ribozyme activities.

Simple mixtures of formic acid and sodium hydroxide, exposed to thermal gradients, drive pH gradients which can be understood and predicted by a separation of timescales. Such proton gradients can locally acid-dissolve Apatite, a presumably abundant phosphate mineral that is close to insoluble at physiological pH. By thermal fractionation, significant concentrations of phosphate are provided at neutral pH.

BP 10.7 Tue 11:30 BAR 0106

Evolution Mechanics: a Framework of Hierarchy Formation

in Evolving Systems — •Yunus Sevinchan — Science of Intelligence Cluster, Technische Universität Berlin, Berlin, Germany — Institute for Theoretical Biology, Humboldt-Universität zu Berlin, Berlin, Germany — Institute of Environmental Physics, Universität Heidelberg, Heidelberg, Germany

The structures we observe around us are of a wide diversity and complexity, ranging from simple cells to intricate ecosystems and human societies. The question how these hierarchically modularized structures can arise from simpler ones is of central importance when desiring to understand our world.

I present the Evolution Mechanics framework [1] which aims to find a concise description of the mechanisms by which evolutionary systems unfold into hierarchically organized modules. Key elements of this conceptual framework are a so-called Self-Replicator and a set of processes that need to occur in order for an Evolutionary Transition in Individuality to take place, thus leading to a new hierarchical level. While inspired by the evolution of biological life, Evolution Mechanics is abstracted from it and takes a more general perspective, providing a consistent language to address the fundamental processes giving rise to the complexity we observe.

[1]: Yunus Sevinchan. Dissertation, 2021. Evolution Mechanics and Perspectives on Food Web Ecology. Heidelberg University Library. DOI: 10.11588/heidok.00030750

BP 10.8 Tue 11:45 BAR 0106

Sequence distributions in coexisting phases — •Ivar Svalheim Haugerud[1], Giacomo Bartolucci[2], and Christoph A. Weber[1] — [1]University of Augsburg, Augsburg, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Phase separation, sequence, and length distributions of heteropolymers such as RNA and DNA are essential in regulating functions and spatial organization in living cells and at the molecular origin of life. Here, we theoretically investigate the interplay between phase separation, polymer sequence, and length at non-dilute conditions. To this end, we developed a thermodynamic description for the reversible polymerization of different monomeric units. In the model, polymers can grow, shrink and phase separate from each other and the solvent. We show that growth in length facilitates phase separation already at low concentrations. Our key finding is that the distribution of sequences is entirely different in each phase. These results suggest that condensed phases can act as hubs for functionalities that rely on the sequence-specificity of RNA or DNA.

BP 10.9 Tue 12:00 BAR 0106

Controlling Alkaline Vent Morphologies in Microfluidic Models by pH and Fluid Flow — •Maximilian Weingart[1], Siyu Chen[2], Clara Donat[2], Dieter Braun[1], and Karen Alim[2] — [1]Systems Biophysics, Ludwig-Maximilians Universität München, Amalienstraße 54, 80799 München, Germany — [2]CPA and Department of Biosciences, School of Natural Sciences, Technische Universität München, Ernst-Otto-Fischer-Straße 8, 85748 Garching b. München, Germany

Alkaline vents provide the unique chemical composition for the precipitation of alkaline fluids in acidic, metal-ion containing ocean water, thereby providing the necessary gradients to drive molecular reactions at the origin of life. Yet, the 3D chimney-like structure of vents pre- vents any visualization of potentially reaction fueling gradients. Here, we develop a microfluidic model of alkaline vents permitting spatio-temporal visualization of precipitate formation and morphology. Varying concentration and inflow rate of an alkaline solution into a flat microfluidic-chamber pre-filled with an acidic Fe(II)-solution we observe a diverse set of precipitate morphologies. Visualizing the precipitation pattern we identify for which physical parameter vent morphologies allow for gradients in pH and molecular composition to arise. We establish our microfluidic model as a framework to investigate the potential of gradients across a permeable boundary for early compartmentalisation and molecular reactions at the Origin of life. The 2D microfluidic alkaline vent model shows that disordered precipitate morphologies allow for the formation of strong pH gradients.

BP 11: Poster Session I

Time: Tuesday 12:30–15:30 Location: P1

BP 11.1 Tue 12:30 P1

Reinforcement Learning: Optimizing Target-search in a homogeneous environment — •Harpreet Kaur, Michele Caraglio, and Thomas Franosch — Institute for Theoretical Physics, Universität Innsbruck, Innsbruck, Austria.

The target-search problem is an interdisciplinary problem comprising several scales, ranging from bacteria looking for food to robots collecting garbage. Generally, in target search we make decisions in an uncertain and often complex environment with the aim of finding a target as efficiently as possible. The key feature that efficient searching agents have in common is the ability to self-propel. Being able to develop efficient search strategies is crucial, as the time needed to discover a target is often a limiting resource. Here, we address the problem of how a smart microswimmer finds a randomly located target in a homogeneous environment by resorting on machine-learning techniques, particularly Reinforcement Learning. We aim to show that learned strategies are optimal and enable minimization of the search time. Also, our work will provide a better understanding of bacteria behavior and biological foraging.

BP 11.2 Tue 12:30 P1

A study of bacteria entrapment using multiparticle collision dynamics — •Pierre Martin and Holger Stark — Technische Universität, Berlin, Germany

The purpose of the current study is to investigate entrapment of bacteria near surfaces. Mechanisms to control trapping of bacteria near solid surfaces is of utmost interest to many medical and biotechnological applications. Trapping leads to enhanced attachement, facilitates the proliferation of cells and ultimately the formation of bacterial biofilms on the surface. Bacteria such as Escherichia coli (E. coli) propel themselves by rotating a bundle of helical flagella. They can change direction by reversing the rotation of a flagella, a process known as tumbling. The motion of bacteria near surfaces induces hydrodynamic interactions with the substract, aligning the cell almost parallel to the surface. This creates an attractive force from the bacteria to the surface, moving and trapping the bacteria along it.

We currently implement a realistic model of E. coli including its tumbling motion within a computer code where we couple it to fluid flow at low Reynolds numbers. The fluid flow is simulated using the method of multi-particle collision dynamics, an efficient solver of the Navier-Stokes equations. Our first goal is to simulate non-tumbling numerical strain of E.coli under shear flow. We will analyse the importance of rheotaxis and Jefferey orbits for near surfaces motility and trapping.

BP 11.3 Tue 12:30 P1

Collective dynamics of multicellular systems in curved geometries — •Tom Brandstätter[1,2], David Brückner[3], YuLong Han[4], Ricard Alert[5], Ming Guo[4], and Chase Broedersz[1,2] — [1]Arnold-Sommerfeld-Center for Theoretical Physics, Ludwig-Maximilians-Universität München — [2]Department of Physics and Astronomy, Vrije Universiteit Amsterdam — [3]Institute of Science and Technology Austria — [4]Department of Mechanical Engineering, Massachusetts Institute of Technology — [5]Max Planck Institute for the Physics of Complex Systems

The multicellular organization of diverse systems, including embryos, intestines, and tumors relies on coordinated cell migration in curved environments. In these settings, cells establish supracellular patterns of motion, including collective rotation and invasion. While such collective modes are increasingly well understood in 2D flat systems, the consequences of geometrical and topological constraints on collective cell migration in 3D curved tissues are largely unknown. Here, we discover a collective mode of cell migration in rotating spherical tissues manifesting as a propagating single-wavelength velocity wave. This wave is accompanied by a pattern of incompressible cellular flow across the spheroid surface featuring topological defects. Using a minimal active particle model, we reveal that this collective mode originates from the active flocking behavior of a cell layer confined to a curved surface. Our results identify curvature-induced velocity waves as a generic ac-

tive matter mode, impacting the dynamical organization of 3D curved tissues.

BP 11.4 Tue 12:30 P1

Self-propulsion of Janus particles at small laser powers and the impact of salt — •Franziska Braun and Regine von Klitzing — Institute for Condensed Matter Physics, Technische Universität Darmstadt, D-64289 Darmstadt

The anisotropy in the architecture allows Janus particles to create an out-of-equilibrium state around the particle in the solvent, which is a necessary condition for triggering self-propulsion. One possible propulsion mechanism is thermophoretic self-propulsion. When laser light (λ = 532 nm) illuminates a gold-capped particle, a local temperature gradient is generated along the particle surface due to surface plasmon excitation of the gold cap. This gradient perturbs the equilibrium conditions of the surrounding medium and leads to self-propulsion.

This contribution focuses on an intensive study of the self-propulsion behavior of self-thermophoretic Janus particles. For this purpose, the movement of the Janus particles is tracked in real-time with dark-field microscopy (DFM). First, the thermophoretic velocity of Au-PS particles is investigated focusing on very low laser powers below 10 mW. Surprisingly, the study shows a deviation of the thermophoretic velocity from the expected linear behavior in the low laser power regime. Secondly, the influence of salt ions on the self-propulsion behavior of such Au-PS particles is described.

BP 11.5 Tue 12:30 P1

An omnipresent material that still suprises: Anomalous stress relaxation of polydimethylsiloxane (PDMS) — Philipp Lach, Erdem Bondan, Pierre-Louis Cramer, Nan Xue, Robert W. Style, Stefanie Heyden, •Charlotta Lorenz, and Eric R. Dufresne — Department of Materials, ETH Zürich, Vladimir-Prelog-Weg 1-5/10, 8093 Zürich, Switzerland

Polydimethylsiloxane (PDMS) is an elastomer which finds ubiquitous use as a model system in experimental settings, as well as in engineering applications. It is easy to fabricate and tune over a large stiffness range. Recent applications in soft robotics have stimulated a closer look at its mechanical properties. Here, we report anomalous responses of PDMS networks to deformation. In one set of experiments, PDMS becomes stiffer after repeated cycles of deformation. In another, PDMS has a non-monotonic stress relaxation in response to a step-strain. Together, these results suggest a mechano-chemical coupling in PDMS where deformed networks are capable of forming new cross-links.

BP 11.6 Tue 12:30 P1

Complex formation between Polyethylenimine and mRNA — •Jonas Lehnen[1], Giovanni Settanni[2], and Friederike Schmid[1] — [1]KOMET 1, Institute of Physics, JGU Mainz, Germany — [2]Faculty of Physics and Astronomy, Ruhr University Bochum, Germany

Messenger RNA vaccines have proven invaluable in the fight against the COVID-19 pandemic. Among the vehicles for non-viral gene delivery Polyethylenimine (PEI) has attracted attention due to its high transfection efficiency. PEI binds to negatively charged mRNA forming polyplexes. These are nanoparticles (NP) of different sizes, depending on the pH used for their assembly as well as salt, PEI and RNA concentration. Small NP have been shown to be critical for high transfection efficiency. We use coarse-grained molecular dynamics simulations to examine the effects of the various factors determining polyplex size and gain a better understanding of the processes involved in their formation, with a special interest on the effects of PEI concentrations way above the amount necessary to neutralize the mRNA, following up on recent experimental results. Experimental and atomistic simulation data were used to tune our model with the aim of finding the mechanism responsible for controlling the size of NPs and give a description of the formation process.

BP 11.7 Tue 12:30 P1

Long-Term Stability, Biocompatibility and Magnetization of Suspensions of Isolated Bacterial Magnetosomes — F. Mickoleit[1], C. Jörke[2], •R. Richter[3], S. Rosenfeldt[4], S. Markert[1], I. Rehberg[3], A. S. Schenk[5], O. Bäumchen[3], D. Schüler[1], and J. H. Clement[2] — [1]Dept. Microbiology, University of Bayreuth, D-95447 Bayreuth, Germany — [2]Dept. Hematology and Medical Oncology, Jena University Hospital, D-07747 Jena, Germany — [3]Experimental Physics V, University of Bayreuth, D-95447 Bayreuth, Germany — [4]Physical Chemistry I, University of Bayreuth, D-95447 Bayreuth, Germany — [5]Physical Chemistry - Collidal Systems, University of Bayreuth, D-95447 Bayreuth, Germany

Magnetosomes are magnetic nanoparticles biosynthesized by magnetotactic bacteria. Due to a genetically strictly controlled biomineralization process, the ensuing magnetosomes have been envisioned as agents for biomedical and clinical applications. In the present work, we examine the stability parameters of magnetosomes isolated from *Magnetospirillum gryphiswaldense* upon storage as a suspension in a buffer solution at 4°C and N_2 atmosphere for one year in the absence of antibiotics. The magnetic potency, measured by the saturation magnetization of the particle suspension [1], drops by 2/3 within this year - about ten times slower than at ambient air and room temperature. The particle size distribution, the integrity of the surrounding magnetosome membrane, the colloidal stability, and the biocompatibility turn out to be not severely affected by long-term storage. — [1] Mickoleit F., et al. (2018). ACS Appl. Mater. Interfaces 10(44), 37898.

BP 11.8 Tue 12:30 P1

The change of DNA radiation damage upon hydration: In-situ observations by near-ambient-pressure XPS — •Marc Benjamin Hahn[1], Paul M. Dietrich[2], and Jörg Radnik[1] — [1]undesanstalt für Materialforschung und -prüfung, Berlin, Germany. — [2]SPECS Surface Nano Analysis GmbH, Berlin, Germany

X-ray photoelectron-spectroscopy (XPS) allows simultaneous irradiation and damage monitoring. Although water radiolysis is essential for radiation damage, all previous XPS studies were performed in vacuum. [1] Here we present near-ambient-pressure XPS experiments to directly measure DNA damage under water atmosphere. They permit in-situ monitoring of the effects of radicals on fully hydrated double-stranded DNA. Our results allow us to distinguish direct damage, by photons and secondary low-energy electrons (LEE), from damage by hydroxyl radicals or hydration induced modifications of damage pathways. The exposure of dry DNA to x-rays leads to strand-breaks at the sugar-phosphate backbone, while deoxyribose and nucleobases are less affected. In contrast, a strong increase of DNA damage is observed in water, where OH-radicals are produced. In consequence, base damage and base release become predominant, even though the number of strand-breaks increases further. [1] Hahn, M.B., Dietrich, P.M. & Radnik, J. In situ monitoring of the influence of water on DNA radiation damage by near-ambient pressure X-ray photoelectron spectroscopy. Commun Chem 4, 50 (2021).

BP 11.9 Tue 12:30 P1

A NAP-XPS-study on X-ray radiation damage: Chemical changes to Gene-V Protein — •Dorothea C Hallier[1,2,3], Jörg Radnik[2], Paul M Dietrich[4], Harald Seitz[1,3], and Marc Benjamin Hahn[2] — [1]Fraunhofer Insitute for Cell Therapy and Immunology, Branch Bioanalytics and Bioprocesses, Potsdam, Germany — [2]Federal Insitute for Materials Research and Testing BAM Berlin, Berlin, Germany — [3]Univerity of Potsdam, Institute for Biochemistry and Biology, Potsdam Germany — [4]SPECS Surface Nano Analysis GmbH, Berlin, Germany

Single-stranded DNA-binding proteins such as Gene-V Protein (G5P/GVP) are involved in maintaining the DNA metabolism after exposure to ionizing radiation, i.e. after radiation therapy in cancer treatment. X-ray photoelectron spectroscopy (XPS) was used to analyze the chemical damage of ionizing radiation to G5P itself. Direct and indirect damage was detected through combined vacuum XPS and near-ambient pressure (NAP) XPS measurements under water and nitrogen atmosphere. The x-ray irridation leads to degradation i.e. via dehydrogenation, decarboxylation, dehydration and deamination. A strong increase of protein damage was observed in water as compared to vacuum.

BP 11.10 Tue 12:30 P1

FTIR and SRE spectra analysis for supported lipids bilayers (SLB's) with dry incorporation of Gramicidin A — •D. Saavedra[1], N. Moraga[1], N. Gomez-Vierling[1], M. Cisternas[2], R. Rodriguez[1], S. Rojas[2], and U.G. Volkmann[1] — [1]Institute of Physics and CIEN-UC, Pontificia Universidad Catolica de Chile — [2]School of Industrial Engineering, Universidad de Valparaiso, Santiago, Chile

A dry method for SLB's assembling was developed in our group, without use of solvents and in vacuum [1], with the aim of synthesizing stable platforms for biosensors. For characterization, FTIR spectrum was analyzed for the detection of functional groups of DPPC and DSPC

phospholipids in the range of 800 - 4000 1/cm. Using the SRE spectrum of DPPC and DSPC, their phase transitions were studied as a function of temperature. The SLB's/Gramicidin interaction at different concentrations were analyzed in order to optimize the growth of the biomolecules. These results would allow to evaluate the use of spin-probes in Gramicidin for the study of ion channel formation [2] and as a prototype for insertion of larger proteins. Acknowledgments: Fondecyt 1180939 (UGV), ANID doctoral grants (NM and NGV) and ANID SIA SA77210032 (MC and SR).

References [1] M. A. Cisternas, et al., Int. J. Mol. Sci. 21 (18), (2020) 6819. [2] Dzikovski, B.G., et al., J. Phys. Chem. B 2011, 115(1), 176-185.

BP 11.11 Tue 12:30 P1

Detection of Gramicidin by DPH fluorescence technique in supported phospholipids bilayers (SLB's) on SiO2 substrate — •D. Saavedra[1], M. Soto-Arriaza[2], N. Moraga[1], N. Gomez-Vierling[1], M. Cisternas[3], and U.G. Volkmann[1] — [1]Institute of Physics and CIEN-UC, Pontificia Universidad Catolica de Chile — [2]Faculty of Medicine and Science, Universidad San Sebastian, Santiago, Chile — [3]School of Industrial Engineering, Universidad de Valparaiso, Santiago, Chile

An unconventional method to manufacture supported lipid bilayers (SLB's) was developed in our laboratory: without solvents, dry [1,2] and in the absence of gases, with the aim of synthesizing stable biosensor platforms. In this work we use our physical fabrication method for the incorporation of specific signal transmitters that have selective sensitivity.

The fluorescence emission spectra of Gramicidin, with DPH as extrinsic probe and fluorescence resonant energy transfer (FRET) techniques, seeks to detect its incorporation into the SLB's.

A series of samples were prepared in absence and presence of Gramicidin and the extrinsic probe DPH. Detection was realized using a single time-correlated spectrofluorimeters photon counting (TCSPC).

Acknowledgments: Fondecyt 1180939 (UGV), ANID doctoral grants (NM and NGV).

References: [1] Cisternas Fruns, M. A. (2021). Ph.D. Thesis, PUC, Chile. https://repositorio.uc.cl/handle/11534/60584. [2] M. A. Cisternas, et al., Int. J. Mol. Sci. 21 (18), (2020) 6819.

BP 11.12 Tue 12:30 P1

Homogenization of DPPC films deposited from the gas phase onto silicon substrates — •N. Moraga[1], D. Saavedra[1], N. Gomez-Vierling[1], M. Cisternas[2], M.J. Retamal[3], and U.G. Volkmann[1] — [1]Institute of Physics and CIEN-UC, Pontificia Universidad Catolica de Chile, Santiago, Chile — [2]School of Industrial Engineering, Universidad de Valparaiso, Santiago, Chile — [3]Engineering Faculty, Universidad Finis Terrae, Santiago, Chile

Supported lipid bilayers (SLBs) are stable structures that allow us to gain insight into the physical behavior of cell membranes through thin film characterization techniques. In this work, DPPC SLBs are made through Physical Vapor Deposition (PVD) technique on silicon substrates without using any solvent [1]. The film thickness was monitored in situ by high-resolution ellipsometry. The DPPC deposition rate, substrate temperature during deposition and post deposition membrane annealing temperature in vacuum and in dry air are used as parameters. Homogeneity of the phospholipid bilayer is observed through the topographical analysis and Young modulus by AFM. Lower deposition rates and a slight increase of substrate temperature led to more homogeneous films. The right annealing temperature and time further improve membrane quality to favor protein insertion [2].

Acknowledgments: Fondecyt 1180939 (UGV) and ANID doctoral grants (NM and NGV)

References:
[1] M. A. Cisternas, et al., Int. J. Mol. Sci. 21 (18), (2020) 6819.
[2] Dzikovski, B.G., et al., J Phys Chem B 2011, 115(1), 176-185.

BP 11.13 Tue 12:30 P1

Foam-like properties of bundled polymer networks — •Lukas Paul Weise, Tobias Alexander Kampmann, and Jan Kierfeld — TU Dortmund University, Germany

We simulate systems of mutually attractive semiflexible harmonic chain polymers in quasi-two dimensions with the event chain algorithm. An isotropic initialization of the system evolves into a network of densely packed bundles of polymers. The resulting structure aims to minimize the overall bundle length which gives rise to properties reminiscent of foams. We examine the applicability of laws and relations characterizing the structure of foams to the bundled polymer networks in order to assess to what extent the networks behave foam-like. The dynamics of the bundled networks are found to be very sensitive with respect to details of the polymer interactions via friction terms albeit qualitative resemblance to foams remains.

BP 11.14 Tue 12:30 P1

Self-assembled Peptides Structure Mediated by Solid Interfaces. — •Leila Sahebmohammadi[1], Regine von Klitzing[1], Markus Mezger[2], and Pol Besenius[3] — [1]Soft Matter at Interfaces, Department of Physics, Technical University of Darmstadt, Hochschulstraße 8, 64289 Darmstadt, Germany — [2]Dynamics of condensed systems, Faculty of Physics, Universität Wien, Währinger Straße 38-42, 1090 Wien, Austria — [3]Department of Chemistry, Johannes Gutenberg-Universität Mainz, Duesbergweg 10-14D-55128 Mainz, Germany

In situ QCM-D reveal a layer-by-layer absorption of the oppositely charged peptides, forming a multilayer. The total amount of adsorbing peptides is derived by the adsorbed temperature and increases with increasing temperature. Exposure to high or low pH (12 or 2) removes the peptide stacks apparently due to reduced electrostatic interaction. AFM result shows the distribution pattern is nanorod-like. These experiments prove stable switchable blocks on the surface that can carry biological and colloidal materials.

BP 11.15 Tue 12:30 P1

Investigations of the Fusion Process of Lipid-Based Nanoparticles with Model Endosomal Membranes Using Coarse-Grained Molecular Dynamics Simulations — •Thomas Kolbe[1], Friederike Schmid[1], and Giovanni Settanni[1,2] — [1]Physics Department, Johannes Gutenberg University Mainz — [2]Faculty of Physics and Astronomy, Ruhr University Bochum

Lipid based nanoparticles have proven to be viable choices for the delivery of genetic material inside a living organism. Compared to the more traditionally used non-pathogenic viruses they attract through potentially much lower costs and milder effects on the immune system. Yet, the exact mechanisms of the endosomal escape - the process with which the delivered drug enters the cell - requires more thorough examination. We simulate the related fusion of a DNA-lipid based nanoparticle with a model endosomal membrane, using coarse-grained molecular dynamics to gain more insights into the underlying processes. By modeling the drop of the system's pH in the various stages of the endosome with different degrees of ionization in our nanoparticle, we can see that the better part of transfections happen at a late stage, confirming that cationic lipids are a main driver of the transfection process. Further, we observe that the size and structure of the nanoparticles have substantial influence on the transfection efficiency.

BP 11.16 Tue 12:30 P1

Machine Learning Guided RNA Contact Prediction — •Utkarsh Upadhyay[1], Oskar Taubert[2], Christian Faber[3], and Alexander Schug[4] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Karlsruher Institut für Technologie, Karlsruhe, Germany — [3]Forschungszentrum Jülich, Jülich, Germany — [4]Forschungszentrum Jülich, Jülich, Germany

For around 50 years, the primary focus of genomic research has been the development of efficient and accurate methods to predict the structure of proteins, which led to the birth of better sequencing techniques and databases. About 98% of the human genome(RNA, DNA) during this action was overlooked.

RNA is not merely a messenger for making proteins, in the past few years, studies have revealed the existence of many non-coding RNAs which catalyse various biological processes; to gain detailed insights into these roles, we require the appropriate structure. Recent years have led to breakthroughs in protein structure prediction via Deep Learning. The scarcity of RNA structures, however, makes a direct transfer of these methods impossible.

We predict contact maps as a proxy to understand and predict RNA structure, they provide a minimal representation of the structure. We have worked on methods that took accuracy from 47%(DCA) to 77%(CoCoNet) and now to 87%(Barnacle). Further, we are trying to create more efficient neural networks for working with limited data, using statistical physics and ML techniques, to substantially reduce the sequence-structure gap for RNA.

BP 11.17 Tue 12:30 P1

Neighbor list artifacts in molecular dynamics simulations —

•Hyuntae Kim — Max Planck Institute for Biophysics — International Max Planck Research School on Cellular Biophysics

Molecular dynamics simulations are widely used in biophysics. To aid non-expert users, most simulation packages provide default values for key input parameters. We found that the default setting of the neighbor list cut-off rlist in the GROMACS package is not sufficient to prevent various artifacts in certain systems. Beyond an already known significant energy drift, we observed catastrophic box deformations of large membrane systems with a semi-isotropically coupled Parrinello Rahman (PR) barostat, rapid oscillations in the pressure, and asymmetric deformations of the box shape. We traced the cause of these artifacts to infrequent neighbor-list updates resulting in missed long-range Lennard-Jones interactions that are systematically attractive. We find that for the small molecular systems commonly simulated, these effects tend to be masked. We present measures to diagnose the problem and guidelines for practitioners.

BP 11.18 Tue 12:30 P1

Sequential resource-sharing speeds up replication in *Plasmodium falciparum* — •Patrick Binder[1,2], Severina Klaus[3], Markus Ganter[3], Ulrich S. Schwarz[2], Thomas Höfer[1], and Nils B. Becker[1] — [1]German Cancer Research Center (DKFZ), Heidelberg — [2]Institute for Theoretical Physics and BioQuant, Heidelberg University — [3]Center for Infectious Diseases, Heidelberg University Hospital

The malaria-causing pathogen *Plasmodium falciparum* is a eukaryotic parasite with a complex life cycle that includes proliferation within red blood cells. After invasion of a red blood cell, the parasite undergoes several rounds of nuclear division and after two days releases around 20 daughter parasites. Although nuclei reside in a shared cytoplasm, using fluorescent imaging, we observe that these cycles desynchronize during multiplication, and do so more rapidly than expected for independent nuclei. To explain the observed asynchrony, we introduce a branching model for allocation of a shared enzyme to the different nuclei. The model encompasses parallel and sequential DNA replication modes. We find that when the shared enzyme is limiting, a sequential replication utilizes resources more efficiently than parallel, which result in faster completion of nuclear multiplication. Overall, our findings suggest that *Plasmodium falciparum* has evolved optimal resource utilization by exploiting a sequential sharing of replication machinery.

BP 11.19 Tue 12:30 P1

Semantic Segmentation for Single Particle Tracking in Noisy Data — •Mattias Luber, Mohammad Amin Eskandari, and Timo Betz — Third Institute of Physics - University of Göttingen

The quantitative analysis of particle motion critically depends on the quality of particle trajectory detection. Especially the position detection of particles in fluorescence microscopy images is an important task faced in biophysics. Trajectories are used to study processes like intracellular transport, protein diffusion within and through membranes and the reconstruction of force fields driving the particle motion. In such settings, high spatial and temporal resolution are desired. However, in practice those factors have contradictory measurement requirements. High temporal resolution requires short exposure times, which limits the photon budget and thus lead to low signal to noise ratios. This work proposes an approach to reconstruct the particle position from noisy images by applying U-NET based deep learning models to fluorescence microscopy images. Further it is shown that this method can successfully track particles with shorter exposure times, compared to traditional approaches.

BP 11.20 Tue 12:30 P1

Mathematical modelling of Nippostrongylus brasiliensis helminth infection: from single worm motility to tissue load dynamics — •Soham Mukhopadhyay[1], Jonathan Pollock[2], David Voehringer[2], and Vasily Zaburdaev[1] — [1]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [2]Department of Infection Biology, University Hospital Erlangen, Friedrich-Alexander University Erlangen-Nuremberg, Germany

Helminth infections affect a large proportion of the world's population and cause significant morbidity. There are no vaccines against helminths, and the mechanisms by which the body fights off helminth infections are not well-understood. To better understand the immune system response we aim to develop a mathematical model describing the helminth load in different organs of the host as a function of time. As an experimental system, we use murine helminth infection by N. brasiliensis worms, where primary, secondary, and infections of mice with altered immune systems could be studied. We model the progression of infection as a system of coupled, time-delayed equations which allow us to link the larvae starting the infection on the skin of mice to the number of eggs shed to the environment by adult worms from the intestine and compare the predictions of the model to the data. For a more microscopic insight into the behaviour of larvae at different developmental stages we carry out biophysical characterisation of larval motility in in vitro settings. Combining these results we aim to achieve a quantitative description of the infection progression in the host.

BP 11.21 Tue 12:30 P1

RNA G-quadruplex folding is a multi-pathway process with a variety of short-lived intermediate states — •Marijana Ugrina[1], Ines Burkhart[2], Diana Müller[2], Harald Schwalbe[2], and Nadine Schwierz[1] — [1]University of Augsburg, Augsburg, Germany — [2]Goethe University, Frankfurt am Main, Germany

The folding kinetics of regulatory RNAs is crucial for their function. Here, we provide molecular insights into the folding pathways of a G-quadruplex from telomeric repeat-containing RNA by combining all-atom molecular dynamics and coarse-grained simulations with circular dichroism experiments. The ion atmosphere surrounding the highly charged quadruplex plays a crucial role in folding. To correctly capture the electric double-layer in implicit solvent coarse-grained simulations, we develop a matching procedure based on all-atom simulations in explicit water. This procedure allows us to provide quantitative agreement between the experiments and simulations as judged by the number of native contacts at different salt concentrations and temperatures. Folding of the quadruplex is on the timescale of minutes and the coarse-grained simulations using the three-interactions site model are therefore ideal to resolve the folding pathways and intermediate states. The results reveal that the folding is sequential with each pathway passing through two transient, on-pathway intermediates: A hairpin and a triplex or double hairpin state. Since these intermediates are degenerate with at two to four alternative conformations per state, quadruplex folding is a multi-pathway process with high conformational entropy.

BP 11.22 Tue 12:30 P1

OCTOPOS.jl: A user-friendly tool for synonymous genetic code optimization — •Simon Christ[1], Jan-Hendrik Trösemeier[2], Christel Kamp[2], and Sophia Rudorf[1] — [1]Leibniz Universität, Hannover — [2]Paul-Ehrlich-Institut, Langen

Synonomous genetic code optimization takes advantage of the fact that aminoacids can be encoded by different nucleotid triplets. It attempts to influence the translation process by synonomous substitutions to alter characteristics such as the protein expression.

OCTOPOS.jl is the reimplementation of the java desktop applicapion OCTOPOS in the julia programming language as a web application.

OCTOPOS combines detailed mechanistic mathematical modeling of in-vivo protein synthesis with machine learning to predict protein expression levels based on codon choice and can generate optimized synonymous mRNA sequences for enhanced heterologous gene expression in different host organisms.

The aim of this reimplementation is to enhance the accessibility of this tool for the community.

BP 11.23 Tue 12:30 P1

Self-regulation of mRNA expression via LNP-based incoherent feed-forward loops — •Judith A. Müller and Joachim O. Rädler — Ludwig-Maximilians-Universität, Munich

Lipid Nanoparticles (LNPs) have revolutionized the delivery of nucleic acid to living cells, including messenger RNAs (mRNAs) and small non-coding RNAs. However, at the single cell level, delivery of LNPs is heterogeneous and the expression level and timing is poorly controlled. A frequently occurring motif in natural gene regulation are incoherent feedforward loops (iFFLs) consisting of simultaneous initiation of activating transcription factors and down-regulating micro-RNAs. Here we realize lipid nanoparticles containing iFFL by ratiometric co-delivery of eGFP coding mRNA and eGFP targeting siRNA. We find faster and more homogenous expression in eGFP time courses using Live Imaging on Single Cell Arrays (LISCA). The steady states levels show power law decrease as a function of siRNA/RNA ratio. Our approach demonstrates self-regulated expression via iFFL-LNP based genetic programs.

BP 11.24 Tue 12:30 P1

How not to lose spikes: inference methods for spike-count neurons — •Tobias Kühn and Ulisse Ferrari — Institut de la Vision, Sorbonne Université, INSERM, CNRS, F-75012 Paris

Maximum-entropy models have been successfully applied to neuronal data stemming from diverse areas like cortex, hippocampus or the retina. Despite this success, it features the major drawback of being restricted to describing every neuron to be in one out of two states: in a given time bin, either there was at least one spike or not. This property does not only limit the statistics that can be matched, but also prevents capturing the neurons' behavior when the firing rate is high, that is when the amount of transmitted information is large. The spike-count model we are suggesting provides a solution to both of these caveats. We are assuming the single-neuron probability distribution to be given in Boltzmann form with energy functions of the shape $E(n) = h \cdot n + J \cdot n^2 + \epsilon \cdot n^3 + \mathcal{O}(n \ln(n))$, where n is the spike count in the respective time bin and ϵ is a small negative hyper parameter guaranteeing that the probability is well-defined for all J. To account for pairwise covariances, we extend the independent neuron case by including an Ising-like interaction term that couples neurons in the network. To infer the model parameters, we develop Monte-Carlo and mean-field methods. We are confident that these techniques will prove useful in the further investigation of neuronal data, in particular in the search for second-order phase transitions.

BP 11.25 Tue 12:30 P1

Parameter Optimization for 1D-0D Coupled Blood Flow Models: Physics-Informed Neural Networks versus Kernel Methods — •Tobias Köppl[1], Benedikt Hoock[1,3], and Gabriele Santin[2] — [1]Technische Universität München, School of Computation, Information and Technology — [2]Digital Society Research Center, Fondazione Bruno Kessler, Italy — [3]Support by Computing Facilities of Leibniz-Rechenzentrum München

The understanding of blood perfusion of organs is essential to improve motion therapy. Here, numerical simulations of the blood flow on the human arteries network have already come up to augment in-vivo measured data. A common approach is the coupled 1D-0D hydrodynamic model combining the simplified incompressible Navier-Stokes equations with the Windkessel model. Fine-tuning the free model parameters such as the resistance and capacity is computationally expensive so it is beneficial to find a simpler surrogate. To this purpose we apply two different machine-learning techniques: physics-informed neural networks and kernel-based methods. The first simultaneously minimizes the quadratic loss to existent reference data and the residuals of a physical system of differential equations by a neural network. The second builds a model from kernel functions and is purely data-driven. We refine these approaches to predict the blood pressure from the 1D-OD model in a single vessel at varying resistance, capacity and heart beat, sampled over time and space. Comparing them in terms of the training and test error and their run time, we conclude that they are equally applicable to be now integrated into quantum optimization.

BP 11.26 Tue 12:30 P1

From in vitro to in silico: a pipeline for the generation of 3D-cell culture simulations from real image data — Elina Nürnberg[1,2,3], Felix Romer[1], •Mario Vitacolonna[2,3], Rüdiger Rudolf[2,3], and Simeon Sauer[1] — [1]Institut für mathematisch-naturwissenschaftliche Grundlagen, Mannheim University of Applied Sciences, Mannheim, Germany — [2]Institute of Molecular and Cell Biology, Mannheim University of Applied Sciences, Mannheim, Germany — [3]Center for Mass Spectrometry and Optical Spectroscopy, Mannheim University of Applied Sciences, Mannheim, Germany

Immunofluorescence labelling, optical tissue clearing and confocal laser scanning microscopy enable the visualization of whole, intact 3D-cell culture models on a single cell level, without loss of 3D spatial information. However, a manual extraction of quantitative information from the entire sample is cumbersome and often only performed on a subset of the data. Moreover, due to lack of computational resources, appropriate statistical methods or theoretical models, this data is often analyzed only qualitatively. In order to overcome these obstacles and improve exploitation of available data beyond quantitative image analysis, we propose a 3D-image analysis pipeline, consisting of image segmentation and 3D-feature extraction to gain quantitative information on cell morphology and protein distribution. Subsequently, this information is used to statistically define prototypical cell types, which are implemented into a basic 3D simulation based on the cellular potts model, which aims to recreate in-silico the in-vitro 3D cell culture, and which can be further adapted to specific research questions.

BP 11.27 Tue 12:30 P1

Determinants of lipid-based nanoparticle structure and stability investigated using molecular dynamics simulations — •Jonas Paulus[1] and Giovanni Settanni[1,2] — [1]Department of Physics, Johannes Gutenberg University Mainz, Germany — [2]Faculty of Physics and Astronomy, Ruhr University Bochum, Germany

mRNA-based therapeutics represent an effective tool to fight several diseases including viral infections, as demonstrated by the COVID-19 vaccination campaign, and cancer. To protect the mRNA from the harsh conditions in a human body, the polyanion is packed into a lipid-based nanoparticle (LNP). This delivery vehicle, although effective, still presents some problems like strict storage requirements, low fraction of successfully delivered mRNA as well as undesirable reactions in some patients. The source of these problems as well as solution approaches are topic of a promising research field. Here we use molecular dynamics simulations to provide a characterization of the internal structure of LNPs and lipid-based nanomaterials for the delivery of RNA. In particular we measure how several observables obtained from different lipid formulations, like the flexibility of bilayers, the tendency to phase separation, the pattern of interactions or behavior under different pH values are related to experimentally measured physico-chemical characteristics as well as to the transfection efficiency. Such structural information could help design more effective lipid formulations for mRNA delivery.

BP 11.28 Tue 12:30 P1

On European Robin cryptochrome 4 interaction with membranes — •Maja Hanic[1], Marta Majewska[2], Izabella Brand[2], and Ilia Solov'yov[1,3,4] — [1]Department of Physics, Carl von Ossietzky University of Oldenburg, Carl-von-Ossietzky Straße 9-11, 26129, Oldenburg, Germany — [2]Department of Chemistry, Carl von Ossietzky University of Oldenburg, Carl-von-Ossietzky Straße 9-11, D-26111, Oldenburg, Germany — [3]Research Centre for Neurosensory Sciences, Carl von Ossietzky University of Oldenburg, Carl-von-Ossietzky Straße 9-11, 26111, Oldenburg, Germany — [4]Department of Physics, Center for Nanoscale Dynamics (CENAD), Carl von Ossietzky University of Oldenburg, Ammerländer Heerstr. 114-118, 26129 Oldenburg

Since the 19th century it was postulated that migratory birds use the geomagnetic field for navigation. Exactly how a migratory bird is able to migrate long distances has become a scientific interdisciplinary question. Recently, cryptochrome 4a from night-migratory songbird European Robin (ErCry4) has been expressed and shown to be sensitive to magnetic field. The sensitivity of ErCry4 to the Earth's magnetic field could be explained by uniform alignment of the ErCry4 protein in bird's eye cells. The possible interaction of ErCry4a with the model membrane mimicking the one found in the outer part of the cone cells was investigated both experimentally and computationally. The experimental and computational results indicate that the ErCry4 does interact with the model lipid membrane. This is the first known observation that ErCry4 interacts with a cell membrane, which could be a key step for ErCry4 to propagate the signal as a magnetoreceptor.

BP 11.29 Tue 12:30 P1

Heat flows through rock cracks purify >50 building blocks of life — •Paula Aikkila, Thomas Matreux, Dieter Braun, and Christof Mast — Systems Biophysics, LMU Munich, Germany

A crucial step during the origins of life is the emergence of biopolymer building blocks. However, the optimal reaction pathways for their formation usually require feedstocks of pure reactants and defined purification and mixing steps to suppress unwanted side reactions and allow for high product yields. We show that heat flows through thin crack-like compartments purify complex mixtures of prebiotically relevant building blocks with high selectivity by bringing together geomaterials, chemistry and microfluidics in a realistic environment. This non-equilibrium process differentially enriches prebiotically relevant building blocks, and distinguishes even mass-identical molecules. Using the experimentally determined thermophoretic properties, we model geologically plausible networks of connected heat flow compartments. Our results show how geologically driven non-equilibria could purify compounds and implement downstream mixing for the origin of life.

BP 11.30 Tue 12:30 P1

Theory of adaptation to a moving optimum — •Sakshi Pahujani and Joachim Krug — Institute for Biological Physics, University

of Cologne, Zülpicher Straße 77, D-50937 Köln, Germany

We study the evolution of a polygenic trait under changing environment using a theory of adaptation formulated by Michael Kopp and Joachim Hermisson [1]. This theory treats the changing environment as a fitness optimum moving in the phenotypic space. Within this framework, we work with the assumption of instantaneous fixation of beneficial mutations. Consequentially, we view adaptation as a walk in the phenotypic space, the dynamics of which are governed by the selection coefficient and the dimensionless speed of the optimum. We investigate the conditions pertaining to the existence of a stationary distribution of the phenotypic lag of the population from the optimum and the dependence of the distribution of adaptive substitutions on the distribution of phenotypic effect sizes available to the population. Further, we go beyond the linear dependence of the optimum on time to non-linear dependencies and incorporate this into the theory to answer questions about the time until first passage through a fitness threshold which potentially leads to the extinction of the population.

[1] Michael Kopp, Joachim Hermisson, genetics.108.099820 (2009)

BP 11.31 Tue 12:30 P1

(De)hydration can speed up chemical process — Ivar Haugerud, •Pranay Jaiswal, and Christoph Weber — Mesoscopic Physics of Life, Institute of Physics, Universitätsstr. 1, Augsburg, Germany

Under early earth conditions, wet-dry cycles and phase separated droplets are separately believed to facilitate chemical processes. Recent experimental studies suggest that chemical reactions can accelerate when subject to non-equilibrium conditions of hydration or dehydration. We develop a theoretical model studying the interplay between wet-dry cycles, phase separation, and chemical processes. We find that hydration and dehydration can significantly increase chemical reaction rates and are further magnified with increasing oscillation amplitudes. Repeated cycles keep the system out of equilibrium, allowing for persistent chemical activity. Furthermore, resonance behaviour in the cycle frequency maximizes the chemical turnover. Our findings show under what conditions the physics of wet-dry cycles could have accelerated chemical reactions in prebiotic soups, similar to enzymes in living cells.

BP 11.32 Tue 12:30 P1

Spontaneous engulfment of microparticles by giant unilamellar vesicles — •Clément Marque and Antonio Stocco — Institut Charles Sadron, Strasbourg, France

Giant unilamellar vesicles (GUVs) are micrometer sized concentric phospholipid bilayers, containing an aqueous medium and constituting simple and controllable model systems to study interaction mechanisms of cells. Adhesion, membrane tension and bending are involved in the engulfment of microparticles and a balance between these contributions is necessary to observe particle wrapping by a GUV membrane. In this context, we mimic the particle endocytosis process by using two types of (1 - 2 microns diameter) colloids interacting with GUVs: uniform silica microparticles and Janus microparticles, half coated with gold nanoparticles (10 - 100 nm) and fabricated by a bottom-up microfluidic self-assembly approach. For this purpose, we aim at controlling particle engulfment in absence of any applied external force. By tuning only membrane properties, we define the critical parameters to observe spontaneous engulfment of microparticles by GUVs. We focus our attention on membrane tension, membrane spontaneous curvature and lipid composition. Membrane spontaneous curvature is tuned by addition of salt, adsorbing onto the outer bilayer surface. Membrane composition is adjusted, as well, to tune lipid fluidity, and membrane surface charge. Finally, Janus microparticle-vesicle interaction will be investigated in out of equilibrium conditions when microparticles are able to self-propel and impart an effective force on the membrane by light exploiting the photothermal properties of gold nanoparticles.

BP 11.33 Tue 12:30 P1

Impact of biomolecular condensates on endocytosis — •Tyler Harmon[1], Max Ferrin[2], and Frank Jülicher[3] — [1]Leibniz Institute for Polymer Research, Dresden, Germany — [2]University of California, Berkeley, USA — [3]Max Planck Institute for the Physics of Complex Systems

Endocytosis is a mechanism that cells use to import material from outside the cell without allowing it immediate access to the cytoplasm. This process involves a section of a cell membrane that is folded inward and then separated into a membrane coated sphere containing the cargo called a vesicle. The process involves recruiting many different protein components to the membrane. We model this recruitment as the formation of a small droplet (biomolecular condensate) located on the membrane. We show using a theoretical model that the presence of a droplet has two major impacts. It creates an additional barrier to initializing endocytosis and it accelerates the process once started. Importantly, the magnitude of this barrier is reduced as droplets get larger. Taken together, droplets are ideal for improving the robustness of endocytosis. It provides a natural checkpoint where cells can ensure they are ready to proceed with endocytosis and, once started, helps ensure that it doesn't stop halfway.

BP 11.34 Tue 12:30 P1

Investigation of thermal fluctuations and elastic properties of lipid bilayers via molecular dynamics simulations — •Clara Rickhoff, Azadeh Alavizargar, and Andreas Heuer — Institute of Physical Chemistry, University Münster, Münster, Germany

As cell membranes consist to a large part of a lipid bilayer and are essential for living cells by forming a barrier between different compartments of cells, which needs to be stable on the one hand but also ductile for processes like cell division on the other hand, the mechanical properties of lipid bilayers are of interest for a better understanding of the behaviour of cell membranes. One important quantity is the bending modulus, which can be extracted from the thermal fluctuation of the bilayer in an equilibrium state and thus from molecular dynamics simulations (MD simulations) and generally can be, due to similar length and time scales, also compared to neutron spin echo spectroscopy (NSE).

In this work, we first performed atomistic MD simulations on a pure DMPC-system and a DPPC-system in order to compare the resulting bending modulus and effective bending modulus with available data from literature. Those simulations were then compared with the results of coarse-grained MD-simulations (CG-simulations), which offer the possibility to examine larger systems and also investigate the impact of transmembrane domains on those quantities.

BP 11.35 Tue 12:30 P1

phospholipids diffusion on the surface of model lipid droplets — •Shima Asfia, Ralf Seemann, and Jean-Baptiste Fleury — Universitüt des Saarlandes, Experimental Physics and Center for Biophysics, 66123 Saarbrücken, Germany

Lipid droplets (LD) are organelles localized in the membrane of the Endoplasmic Reticulum (ER) that play an important role in metabolic functions. Many studies have focused on the biophysical properties of these LDs. However, despite numerous efforts, we are lacking information on the mobility of phospholipids on the LDs surface, although they may play a key role in the protein distribution. In this article, we developed a microfluidic setup that allows the formation of a triolein*buffer interface decorated with a phospholipid monolayer. Using this setup, we measured the motility of phospholipid molecules by performing Fluorescent Recovery After Photobleaching (FRAP) experiments for different lipidic compositions. The results of the FRAP measurements reveal that the motility of phospholipids is controlled by the monolayer packing decorating the interface [1].

[1]S. Asfia, R. Seemann and J-B. Fleury, BBA-Biomembranes, 1865, 1 (2023).

BP 11.36 Tue 12:30 P1

SAXS measurements during polychromatic illumination of photoswitching in azobenzene lipid vesicles — •Matthias Lösche[1], Benedikt Baumgartner[2], Benjamin Ajanovic[1], Oliver Thorn-Seshold[2], and Bert Nickel[1] — [1]Faculty of Physics and CeNS, Ludwig-Maximilians-Universiät München, Geschwister-Scholl-Platz 1, Munich 80539, Germany — [2]Department of Pharmacy, Ludwig-Maximilians-Universität München, Butenandtstraße 5-13, Munich 81377, Germany

Photoswitchable molecules are envisioned to be used in the field of nanomedicine. Here we study photoswitchable azobenzene lipids which switch to predominantly cis-state at 365 nm wavelength illumination and to trans-state at 465 nm illumination. The conformational change of the lipid induces different vesicle membrane thicknesses, which can be read out by small-angle x-ray scattering, as established by us before. What is not yet known is how azobenzene lipid vesicles behave when irradiated at other wavelengths. We illuminate lipid vesicles with 16 different wavelengths (generated by high-power LEDs) which cover the whole visible light region. We follow the kinetics of the switching process by SAXS. This establishes an action spectrum that correlates the different photostationary states with illumination wavelength.

BP 11.37 Tue 12:30 P1

Two-photon 3D laser printing inside synthetic cells — •Tobias Abele[1,2], Tobias Messer[3], Kevin Jahnke[1,2], Marc Hippler[3], Martin Bastmeyer[3], Martin Wegener[3], and Kerstin Göpfrich[1,2] — [1]Max Planck Institute for Medical Research, Heidelberg, Germany — [2]Heidelberg University, Heidelberg, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany

Towards the ambitious goal of manufacturing synthetic cells from the bottom up, various cellular components have already been reconstituted inside of lipid vesicles. However, the deterministic positioning of these components inside the compartment has remained elusive. Here, by using two-photon 3D laser printing, 2D and 3D hydrogel architectures were manufactured with high precision and nearly arbitrary shape inside of preformed giant unilamellar lipid vesicles (GUVs). The required water-soluble photoresist is brought into the GUVs by diffusion in a single mixing step. Crucially, femtosecond two-photon printing inside the compartment does not destroy the GUVs. Beyond this proof-of-principle demonstration, early functional architectures were realized. In particular, a transmembrane structure acting as a pore was 3D printed, thereby allowing for the transport of biological cargo, including DNA, into the synthetic compartment. These experiments show that two-photon 3D laser microprinting can be an important addition to the existing toolbox of synthetic biology.

BP 11.38 Tue 12:30 P1

Self-patterning of polyelectrolyte multilayer films: the roles of PSS molecular weight, the top layer, and post-preparation treatment — Amir Azinfar and •Christiane A. Helm — Institute of Physics, University of Greifswald, Germany

The self-patterning of thin films is relevant both for fundamental research and applications. We investigate polyelectrolyte multilayer films made from poly(diallyldimethylammonium) and poly(styrene sulfonate) (PDADMA/PSS). Various PSS with low molecular weight were used. Invariably, the film thickness increases exponentially with the number of deposited PDADMA/PSS bilayers. The separation and height of the domains increase significantly with each deposited PDADMA/PSS bilayer, as AFM images show. At the end of the exponential growth regime, either a parabolic (and then a linear) or a linear growth regime follows, depending on the selected PSS molecular weight. In the non-exponential growth regimes, the domain separation changes less during film growth than in the exponential growth regime.

PSS is more strongly bound to the film than PDADMA. PSS-terminated films show the same domain distance in water and air. However, when PDADMA-terminated films are dried, the domain distance in the air increases while the domain height decreases, causing a reduction in total area. In the air, the surface energy is greater than in water, and a highly textured surface costs a lot of energy. We propose the changed surface pattern is attributable to energy minimization. Furthermore, the domains are stable when exposed to 1 M NaCl solution but shrink in 2 M NaCl.

BP 11.39 Tue 12:30 P1

Membranes with large phospholipid asymmetries — •Martin Girard — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz

Plasma membranes in cells are asymmetric, an observation that dates 40 years. Recent observations suggest that these membranes present large lipid number asymmetries, with almost twice as many phospholipids on one of the leaflet than the other. Simulations provide an excellent avenue to probe behavior of these membranes. Here, I discuss the behavior of such membranes, in particular with respect to chemical asymmetries in the membrane. The work required to establish the phospholipid number asymmetry is also discussed, a quantity that is directly related to the work done on lipids by the so-called flippases and floppases proteins responsible for asymmetry homeostasis.

BP 11.40 Tue 12:30 P1

Wetting-effects of liquid-liquid condensates on lipid membranes — Chae Yeon Kang, Yoohyun Chang, and •Katja Zieske — Max Planck Institute for the Science of Light, Erlangen

Liquid-liquid condensates are supramolecular assemblies of proteins and RNA molecules and have been studied extensively, due to their ability to spatially structure cells and to spatially confine biological reactions. However, little is known about the interactions of liquid-liquid condensates with lipid membranes and the consequences of these interactions on cellular length scales.

Here, we used a cell-free bottom-up approach to reconstitute liquid-liquid condensates at lipid membranes. Our results demonstrate how lipid membranes and liquid-liquid condensates interact under various experimental conditions and point towards an important role of wetting-effects in intracellular organization.

BP 11.41 Tue 12:30 P1

A preparative mass spectrometer to deposit intact large native protein complexes — •Paul Fremdling[1], Tim K. Esser[1], Bodhisattwa Saha[1], Alexander A. Makarov[2,3], Kyle L. Fort[2], Maria Reihnhardt-Szyba[2], Joseph Gault[1], and Stephan Rauschenbach[1,4] — [1]Chemistry Research Laboratory, University of Oxford, 12 Mansfield Road, Oxford OX1 3TA, UK — [2]Thermo Fisher Scientific, Bremen, 28199, D — [3]Bijvoet Center for Biomolecular Research, University of Utrecht, Padualaan 8, 3584 CH Utrecht, NL — [4]MPI for Solid State Research, Heisenbergstrasse 1, Stuttgart, 70569, D

Electrospray ion-beam deposition (ES-IBD) is a tool to study structure and reactivity of nonvolatile molecules. It ionises molecules gently, purifies and deposits them onto a substrate. In combination with imaging techniques, direct structural information can be obtained.

There are only a small number of custom ES-IBD instruments worldwide, with no commercial ones. We present a module that adds ion-beam deposition capabilities to a commercial MS (Thermo ScientificTM Q ExactiveTM UHMR).

We characterise beam intensity, landing-energy control, and deposition spot size for a broad range of molecules. In combination with atomic force microscopy (AFM) and transmission electron microscopy (TEM), we distinguish near-native from unfolded proteins and show retention of native shape of protein assemblies after dehydration and deposition. Further, we use an enzymatic assay to quantify activity of a non-covalent protein complex after deposition on a dry surface.

BP 11.42 Tue 12:30 P1

Tracking the Electron Transfer Cascade in European Robin Cryptochrome 4 Mutants — •Daniel Timmer[1], Anders Frederiksen[1], Daniel C. Lünemann[1], Anitta R. Thomas[1], Jingjing Xu[1], Rabea Bartölke[1], Jessica Schmidt[1], Tomas Kubar[2], Antonietta De Sio[1], Ilia A. Solov'yov[1], Henrik Mouritsen[1], and Christoph Lienau[1] — [1]University of Oldenburg, Germany — [2]Karlsruhe Institute of Technology, Germany

The ability of some birds to sense weak earth-strength magnetic fields for navigation is thought to rely on the quantum mechanical radical pair (RP) mechanism [1]. Here, cryptochrome proteins, located in the birds retina, can undergo consecutive electron transfers after blue light photo-excitation of a bound flavin chromophore with a nearby chain of four tryptophan amino acid residues. This leads to the formation of a long-lived RP, which can interconvert between the singlet and triplet state due to hyperfine interactions. Spin-selective signaling state populations can eventually be influenced via a weak external magnetic field [1]. Using pump-probe spectroscopy on wildtype cryptochrome protein of the European robin and a series of mutants, where we selectively blocked the electron transfer along the chain with redox-inactive phenylalanine, we are able to track RP formation step by step and extract the electron transfer times and yields [1]. Our experimental study is supported by theoretical modeling of the electron transfer cascade using a mixed quantum mechanical/molecular mechanical approach. [1]: Xu, Jingjing, et al., Nature 594.7864, 535-540 (2021). [2]: Timmer, Daniel, et al., arXiv preprint arXiv:2205.10393 (2022).

BP 11.43 Tue 12:30 P1

Nonlinear Transmission of FUS Protein Solution at 0.5 THz — •Quang Minh Thai[1], Igor Ilyakov[2], Manthan Raj[1], Daniel Dornbusch[2], Atiqa Arshad[2], Thales de Oliveira[2], Marcus Jahnel[1,3], Jan-Christoph Deinert[2], Alexey Ponomaryov[2], Sergey Kovalev[2], and Ellen M. Adams[1,2] — [1]Cluster of Excellence Physics of Life (PoL), TU Dresden, Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — [3]Center for Molecular and Cellular Bioengineering, Biotechnology Center, TU Dresden, Dresden, Germany

Water possesses strong absorption in the THz range due to intermolecular vibrational modes in a network of hydrogen-bonded water molecules. Its THz response is also sensitive to the coupling of water to other molecules, i.e. the hydration shell of a protein. Probing the nonlinear properties of hydration water can provide insight into protein solvent dynamics, and in the case of intrinsically disordered proteins, its subsequent role in the liquid-liquid phase separation (LLPS). Such

characterization at low THz frequencies (< 3 THz) remains yet limited, due to the scarcity of brilliant light sources in this range. Here, we present the nonlinear characterization at 0.5 THz of water and FUS protein solution in a liquid transmission cell, using a THz time-domain spectroscopy (THz-TDS) setup with the TELBE free electron laser source at HZDR. Our results show that the nonlinear absorption and refractive indices of the FUS protein solution differ from that of water, indicating a perturbed hydrogen bonding network.

BP 11.44 Tue 12:30 P1

Bio-SAXS of Single-Stranded DNA-Binding Proteins: Radiation Protection by the Compatible Solute Ectoine — •Marc Benjamin Hahn[1], Dorothea C. Hallier[1,2,3], Glen J. Smales[2,3], and Harald Seitz[1] — [1]Bundesanstalt für Materialforschung und prüfung (BAM), 12205 Berlin, Germany — [2]Fraunhofer Institute for Cell Therapy and Immunology, Branch Bioanalytics and Bioprocesses (IZI-BB), 14476 Potsdam, Germany — [3]Universität Potsdam, Institut für Biochemie und Biologie, 14476 Potsdam, Germany

Small-angle X-ray scattering (SAXS) can be used for structural determination of biological macromolecules and polymers in their native states. To improve the reliability of such experiments, the reduction of radiation damage occurring from exposure to X-rays is needed.One method, is the use of scavenger molecules that protect macromolecules against radicals produced by radiation exposure.In this study we investigate the feasibility to apply the compatible solute, osmolyte and radiation protector Ectoine (THP(B)) as a scavenger throughout SAXS measurements of single-stranded DNA-binding protein Gene-V Protein (G5P/GVP). Therefore we monitor the radiation induced changes of G5P during bio-SAXS. The resulting microscopic energy-damage relation was determined by particle scattering simulations with TOPAS/Geant4. The results are interpreted in terms of radical scavenging as well as post-irradiation effects, related to preferential-exclusion from the protein surface. Thus, Ectoine provides an non-disturbing way to improve structure-determination of proteins via bio-SAXS in future studies.

BP 11.45 Tue 12:30 P1

Molecular Dynamics Simulations of Large Proteins in Vaccum and during Surface Adsorbtion — •Alpcan Önür[1,2], Tim K. Esser[2], Christoph Globisch[1], Christine Peter[1], and Stephan Rauschenbach[2,3] — [1]Departement of Chemistry, University of Konstanz, Konstanz, Germany — [2]Departement of Chemistry, University of Oxford, Oxford, UK — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany

Knowledge of protein structures is crucial for biological and medical research in for instance metabolism, drug discovery and diseases. Cryogenic electron microscopy (cryo-EM) recently became a dominant method of protein structure determination. One of the main challenges with cryo-EM measurements lies in the protein preparation with many pitfalls which can destroy the native structure of proteins due to surface effects. The combination of electrospray ion beam deposition (ESIBD) and native mass-spectrometry creates chemically selective cryo-EM samples. This method has the potential to overcome many conventional cryo-EM sample preparations. However, the native ESIBD-CryoEM approach prepares and images dehydrated gas-phase proteins, which have collided with a surface. This can affect the native protein fold and hence influence the cryo-EM obtained structure, for instance reducing the resolution or inducing deviations. In this work we will present first steps towards understanding structural changes of proteins in electrospray ion beams, after surface interactions, and during dehydration in ultra-high vacuum by utilizing molecular dynamics simulations.

BP 11.46 Tue 12:30 P1

Dynamics of Tau protein studied with X-ray photon correlation spectroscopy (XPCS) — •Sebastian Retzbach[1], Nimmi Das Anthuparambil[2,5], Anita Girelli[3], Kevin Pounot[4], Sonja Timmermann[2], Maximilian D. Senft[1], Marvin Kowalski[2], Michelle Dargasz[2], Nafisa Begam[1], Fabian Westermeier[5], Anastasia Ragulskaya[1], Fajun Zhang[1], Christian Gutt[2], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Universität Siegen, Germany — [3]Stockholm University, Sweden — [4]ESRF, Grenoble, France — [5]DESY, Hamburg, Germany

Proteins exhibit a rich phase behavior, including the formation of amyloid fibrils, which have been linked to many diseases, e.g. Alzheimer's disease. Understanding the dynamics associated with amyloid fibril formation and beyond, such as liquid-liquid phase separation, nucleation and gel-formation, is thus of substantial interest. X-ray photon correlation spectroscopy (XPCS) is a state-of-the-art method to study matter over a broad range of time- and length scales, which was successfully used to study protein systems [1]. Here, we use this method to follow the dynamics and the structural changes of the Alzheimer associated, amyloid fibril forming, protein Tau. After inducing the fibrillation with Heparin, at a Tau concentration of 100 mg/ml, and waiting for 22 hours, a fractal structure with a characteristic length of around 200 nm has evolved. The dynamics exhibited ballistic behavior that show similarities to the dynamics in gels.

[1] A. Girelli et al. (2021) Phys Rev Lett 126, 138004.

BP 11.47 Tue 12:30 P1

Upconversion-nanoparticle optical trapping for ultraresolution motor protein measurements — •Aleksandr Kostarev and Erik Schäffer — Universität Tübingen, ZMBP, Tübingen, Deutschland

Molecular machines are essential for many cellular processes. For example, kinesin motor proteins transport cargo along microtubule cytoskeletal filaments. The stepping and force generation of single motors can be measured using optical tweezers. However, the spatiotemporal resolution achieved with common optical tweezers probes is insufficient to detect fast steps in particular at low forces. To improve the resolution, nanoparticles are required as optical tweezers probes. Upconversion nanoparticles trapped near resonance of their electric susceptibility have the highest reported trapping efficiency and are chemically stable. Yet, they have not been used for biophysical measurements. To use them, we have integrated a near-resonance trapping laser, detector, and laser steering system in an optical tweezers system. Calibration measurements show that the upconversion nanoparticles indeed have a very high trapping efficiency when trapped with a laser near resonance compared to off-resonance trapping. Once functionalized with the motors, trapping experiments will shed light on how weak kinesin motors step and diffuse on microtubules. In the long term, upconversion-nanopartical optical trapping will improve the spatiotemporal resolution of optical tweezers and shed light on the working mechanism of a wide range of molecular machines.

BP 11.48 Tue 12:30 P1

Diffusive anchorage of molecular motors facilitates robust cargo transport — •Rachele Catalano[1], Gina A. Monzon Monzon[1,2], Rahul Grover[1], Ludger Santen[2], and Stefan Diez[1,3] — [1]B CUBE - Center for Molecular Bioengineering, TU Dresden — [2]Center for Biophysics, Department of Physics, Saarland University — [3]Cluster of Excellence Physics of Life, TU Dresden

Intracellular transport of vesicles and organelles is carried out by teams of molecular motor proteins moving cargo along polar intracellular filaments. Multiple-motors are coupled to each other via a fluid membrane that allows motors to diffuse along the cargo surface. How the number of involved motors and the diffusivity of motors on the cargo surface influence such transport is not well understood. Here we use a combined experimental and theoretical approach to investigate the impact of motor number and motor-cargo interaction on the motility parameters of kinesin-driven cargoes moving along microtubules. We found that the velocities of cargoes with highly diffusive motors decrease with an increase in motor number. Cargoes with non-diffusively bound motors moved with velocities independent of the motor number. Numerical simulations reveal that diffusive motor-cargo binding results in higher numbers of microtubule-bound motors, which increases steric hindrance associated with cargo slow down. Additionally, the higher number of microtubule bound motors enhances cargo run length and increases transport robustness. Our results demonstrate that loose mechanical coupling of multiple motors by diffusive membrane anchorage leads to robust transport at the cost of lower velocity.

BP 11.49 Tue 12:30 P1

Amplified self-stabilization of cell adhesions under load — •Julia Müllner[1,2] and Benedikt Sabass[1,2] — [1]Institute for Infectious Diseases and Zoonoses, Department of Veterinary Sciences, LMU München — [2]Department of Physics, LMU München

Cell adhesion is crucial for the structural organization of living organisms. Experimentally, it was found that planar cell-matrix adhesions respond to an increase in shear force by growing in size in order to maintain structural stability. As part of this process, the protein vinculin binds to force-activated binding sites of talin and to actin, thereby strengthening the cluster. However, it is not fully understood how mechanical forces induce adhesion molecules to drive adhesion

growth. We present a minimalist model to explore the dynamics of an adhesion cluster under shear force. The system is reduced to a single adapter molecule species (talin) that can undergo conformational changes when being stretched. As in an open system, molecules are exchanged between a reservoir and the adhesion cluster. To account for adhesion growth upon molecule unfolding, we expand the reservoir rate to be proportional to the number of unfolded molecules. Simulation results show that the number of adhesion bonds rises with increasing shear force, as seen in experiments. A state diagram is constructed, delineating regimes of adhesion stabilization from unbounded growth and adhesion rupture. An analytical mean-field model yields solutions that are in good agreement with the simulation results. Overall, we describe and characterize a mechanism that amplifies self-stabilization of cellular adhesions under load.

BP 11.50 Tue 12:30 P1

Is sensory adaptation generally limited by the energy-speed-accuracy tradeoff? — •Vansh Kharbanda[1,2] and Benedikt Sabass[1,2] — [1]Institute for Infectious Diseases and Zoonoses, Department of Veterinary Sciences, LMU München — [2]Department of Physics, LMU München

Sensory adaptation is vital to all living organisms. An adaptive sensory system can be modelled as a stochastic, nonlinear feedback network. Using a generic framework, we study the accuracy of adaptive mechanisms and its energetic cost. Recently, it has been suggested that the steady-state dissipation rate associated to maintenance of an adaptive state increases logarithmically with the adaptation accuracy. We present results that demonstrate that this logarithmic scaling does not hold generally, but appears to be linear when the state of the system is close to the phase-space boundaries. Our numerical results also suggest that boundaries in the phase space of system variables limit the capacity of the system to dissipate. Moreover, we conjecture a new empirical expression relating the steady-state dissipation rate and the strength of the input signal if the state lies in the vicinity of the boundaries. Finally, the combined adaptation accuracy of two linearly coupled systems is studied. We show that a coupling of the outputs of the systems deteriorates the overall adaptation accuracy while the associated energy cost is also reduced. In contrast, a coupling of the control elements reduces the dissipation rate without compromising on the adaptation accuracy.

BP 11.51 Tue 12:30 P1

Three-compartment model describes coarsening of biomolecular condensates in Meiosis — •Marcel Ernst and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

During meiosis, crossovers between the female and male chromosomes mix genetic information. Experimental observations consistently reveal two key findings: First, the number of crossovers per chromosome is at least one and usually small, between one and three. Second, there is crossover interference, which prevents nearby crossovers on a single chromosome. A recently suggested model proposes biomolecular condensates that coarsen by exchanging material along chromosomes to determine crossovers. We extend this model by including the exchange with the surrounding nucleoplasm, leading to a three-compartment model. We validate the model by comparing numerical results with various experimental data in Arabidopsis. In particular, we explain the behavior of a mutant without the axial structure linking the chromosome pairs. Moreover, we derive scaling laws, analogous to Lifshitz-Slyozov-Wagner theory, predicting the final number of crossovers, and their spatial structure as a function of coarsening time, chromosome length, and the initial amount of material. In summary, our model reveals how meiotic crossovers are regulated in wild-type and in mutants.

BP 11.52 Tue 12:30 P1

Investigation on the learning ability of the single-celled slime mould *P. polycephalum* — •Adrian Büchl, Lisa Schick, and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

The slime mould *Physarum polycephalum* is well known for its ability to store information and perform complex problem-solving despite being just a single, gigantic, network-shaped cell. Yet, can we consider such complex behaviour learning? Using bright-field microscopy observations we investigate how *P. polycephalum* networks react to repetitive negative blue light stimuli. We vary stimuli duration and the concentration of the growth medium in the substrate to probe how training time and migration speed impact *P. polycephalum*'s ability to follow trained behaviour.

BP 11.53 Tue 12:30 P1

Can iron-phthalocyanines, Fe-Pc, on CrI3 imitate active site of hemoglobin? — •Cihan Bacaksiz and Maria Fyta — Computational Biotechnology, RWTH Aachen University, Aachen, Germany

The metallo-phthalocyanines (M-Pc) molecules are studied for their chemical, magnetic, and optoelectronic properties. They can function in a wide range of applications, such as gas sensors, field effect transistors, organiclight-emitting diodes, and data storage devices. More specifically, the core of iron-phthalocyanines (Fe-Pc) resembles structurally the active site of hemoglobin (heme), which is responsible of holding the oxygen and carbon dioxide. Motivated by this potential, we have studied the oxygen-capture and -release properties of Fe-Pc on top of magnetic monolayer CrI3 using first-principle simulations. The interplay between the magnetic properties of Fe-Pc on CrI3 and its chemical activity are investigated. It is found that the surface effects on the molecule accompanied with the magnetic interactions between Fe and Cr atoms can be used to manipulate - even control - the oxygen capture-release properties of Fe-Pc.

BP 11.54 Tue 12:30 P1

Band formation of red blood cells by density gradient centrifugation — •Luca David Hastenteufel, Felix Milan Maurer, and Christian Wagner — Experimentalphysik, Universität des Saarlandes, Saarbrücken

Percoll is a commercial density medium consisting of coated silicia particles, which show a non-toxiticy to cells and low surface charge. Nowadays, Percoll is the standard medium for density separation of erytrocytes, leukocytes and other subcellular particles. The distribution of red blood cells after centrifugation in a self-forming Percoll gradient is characterized by a heterogeneous structure of discrete bands. We established a one dimensional particle model and a set of experiments to show that band formation is caused by aggregation. We also developed a continuum model describing the development of the RBC volumetric density under influence of a pair interaction. It shows also discrete solutions in the shape of band patterns. Understanding the band patterns gives information on the aggregation energy and disease severeness.

BP 11.55 Tue 12:30 P1

Exploiting Onsager regression in passive measurements to reveal active mechanics of living systems — Till Muenker, Gabriel Knotz, Matthias Krüger, and •Timo Betz — Faculty of Physics, Georg-August-University Göttingen

Understanding life is arguably among the most complex scientific problems faced in modern research. From a physics perspective, living systems are complex dynamic entities that operate far from thermodynamic equilibrium. This active, non-equilibrium behaviour, with its constant hunger for energy, allows life to overcome the dispersing forces of entropy, and hence drives cellular organisation and dynamics at the micrometer scale. Unfortunately, most analysis methods provided by the powerful toolbox of statistical mechanics cannot be used in such non-equilibrium situations, forcing researchers to use sophisticated and often invasive approaches to study the mechanistic processes inside living organisms. Inspired by Onsager's regression hypothesis, we introduce here a Mean Back Relaxation (MBR) observable, which detects active motion in purely passive measurements of particle fluctuations. The MBR, which is based on three point probabilities, is theoretically and experimentally shown to exhibit markers of non-equilibrium, i.e., of detailed balance breaking dynamics. We furthermore observe an astonishing relation between the MBR and the effective non-equilibrium energy in living cellular systems. This is used to successfully predict the viscoelastic response function and the complex shear modulus from a purely passive approach, hence opening the door for rapid and simple passive mechanics measurements even in active systems.

BP 11.56 Tue 12:30 P1

Theory of rheology and aging of protein condensates — •Ryota Takaki[1], Louise Jawerth[2], Marko Popovic[1], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Leiden University

Biological polymeric materials form liquid droplets through liquid-liquid phase separation, referred to as biological condensates. Although the material properties of biological condensates are deemed to

play essential roles in cellular functions, quantitative studies of condensates' rheology became available very recently. Particularly the experiments found the glass-like material property of condensates, showing slow relaxation, termed "aging" in the glass field. In this study, we develop a rheological model of biological condensates from the physical pictures: diffusion and stochastic binding of proteins inside condensates. We obtain the constitutive equation for the material property of protein condensates showing aging behavior observed in experiments. We elucidate how aging manifests in the experimental observations in microrheology, both in active and passive rheology. We develop a novel method for active rheology to compute the time-dependent property of aging materials. We derive generalized fluctuation-response relations to bridge the mean squared displacement of diffusing elements inside aging Maxwell fluid to the time-dependent material properties, which can be used in passive rheology.

BP 11.57 Tue 12:30 P1

Mitochondrial dynamics control cellular anti-viral responses in the innate immune system — •Felix J. Meigel[1] and Steffen Rulands[2,1,3] — [1]MPI for the Physics of Complex Systems, Dresden, Germany — [2]Arnold Sommerfeld Center for Theoretical Physics, Department of Physics, Ludwig-Maximilians-Universität, München, Germany — [3]Center for Systems Biology Dresden, Germany

The inflammation response of mammalian cells to infection with RNA viruses (e.g. coronaviruses or influenza A) is mediated by the signaling pathway around the protein MAVS. For an efficient inflammation response, MAVS proteins need to form large homo-oligomers on the mitochondrial membrane. Here, we discuss how mitochondrial fusion and fission assists the formation of large membrane-bound protein aggregates by inducing density fluctuations among mitochondria. We demonstrate how the dynamic compartmentalization of the protein aggregation dynamics by steady organelle fusion and fission qualitatively alters the extreme value statistics of the aggregate size distribution beyond a limit set by the Vigil-Ziff criterion. We develop a thermodynamic framework, that allows us to asses under which conditions dynamic compartmentalization affects the aggregate size distribution and facilitates the formation of large aggregates. In this work, we not only emphasize the importance of mitochondrial dynamics for efficient immune responses but also introduce a framework to discuss the non-equilibrium thermodynamics of multi-scale systems in the context of dynamic compartmentalization.

BP 11.58 Tue 12:30 P1

Monodominance in tropical forests: modelling the influences of biological mechanisms on cluster formation — •Julia Meyer[1], Pia Backmann[2], and Alexander K. Hartmann[1] — [1]Institute of Physics, University of Oldenburg, Germany — [2]University of Leipzig, Germany

Monodominance in tropical forests describes the formation of patches dominated by a single tree species, i.e., *clusters*, in an otherwise highly species-rich forest. The reasons for its emergence are not fully understood yet, probably multiple causes exist [1], depending on the specific forest.

Recently, a statistical-mechanics model was introduced [2] which allowed for an analysis of the cluster formation process. A phase transition between a non-percolating and a monodominated percolating phase could be observed, and analyzed by finite-size scaling techniques. The properties of this system, such as the morphology of clusters, are quite distinct from standard percolation. Here, we numerically [3] further investigate extensions of the model by including different biological mechanisms, like shade tolerance, that are believed to potentially favor monodominance. We analyze how the properties of this phase transition change for the modified model.

[1] K. S.-H. Peh, S.L. Lewis, and J. Lloyd, J. Ecol. **99**, 891 (2011).
[2] M. Kazmierczak et al., J. R. Soc. Interface **13**, 20160123 (2016).
[3] A.K. Hartmann, *Big practical Guide to Computer Simulations* (World Scientific, 2015).

BP 11.59 Tue 12:30 P1

Phase segregation and microemulsion module of DNA oligo based nano-motifs — •Rakesh Chatterjee[1], Mai P. Tran[2], Yannik Dreher[2], Julius Fichtler[2], Kevin Jahnke[2], Xenia Tschurikow[3], Aaron Gadzekpo[3], Lennart Hilbert[3], Kerstin Göpfrich[2], and Vasily Zaburdaev[1] — [1]Friedrich-Alexander- Universität Erlangen-Nürnberg, Germany — [2]Max Planck Institute for Medical Research, Heidelberg, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany

DNA can be used as a programmable material by designing the base sequences to drive self-assembly. The technology of forming macromolecular droplets through sequence design of DNA-like biopolymers could provide insights into the mechanisms of liquid-like droplet formation via liquid-liquid phase separation. In two experimental setups we study how the process of phase segregation of two motifs is affected by confinement and how the dispersal of the aggregated phase is controlled by addition of amphiphiles. To quantify this process theoretically we use a versatile lattice-gas model in two dimensions with cross-shaped particles that can closely mimic the shape of synthetic nano-motifs and their interaction valencies as well as account for their translational and rotational diffusion. With our numerical results we can recapitulate the observed effects of the slowing down phase segregation in confinement and the dose response of the aggregate dispersal by addition of amphiphile components.

BP 11.60 Tue 12:30 P1

Delay time of erythrocyte sedimentation rate — •Jan Fischer, Thomas John, Lars Kaestner, Christian Wagner, and Alexis Darras — Experimental Physics, Saarland University; D-66123 Saarbrücken, Germany

In many suspensions of microscopic particles, ranging from cosmetic creams to food dough to oil paints, the suspended sate is only transient. Indeed, unless the densities of particles and fluid are perfectly matched, gravity eventually separates the two phases. In many practical cases with a high concentration of particles, this separation happens as a sudden "collapse" after a long period (sometimes months or years) where no separation was observed. This phenomenon actually defines the life span of many practical products.

Our group recently demonstrated that red blood cells (aka erythrocytes) follow the same behavior on short time scales. This has practical application, since their average sedimentation rate is used as a medical parameter. However, while it is known that the collapse delay time has an intrinsic random component for thermal suspensions, it is not clear whether it is the case for red cells, which are mainly athermal.

For the first time, we characterized the variability of the delay time for a given suspension of red blood cells. Moreover, the influence of various parameters unique to red blood cells, such as cell shape and rigidity, has been studied and correlated with the microstruture of the red blood cells aggregates.

BP 11.61 Tue 12:30 P1

Modeling of protein condensates — •Kathrin Hertäg and Joshua Robinson — ITP4, Stuttgart, Deutschland

Phase separation in systems driven away from thermal equilibrium has recently attracted substantial interest, in particular for motile active matter and protein condensates in cells. The latter are characterized by a finite size that can be stable *in vivo* over the whole cell cycle while *in vitro* the same proteins undergo conventional phase separation that coarsens towards a fully phase-separated state. The physical processes that control the condensate size are largely unexplored. Here we apply methods from active liquid theory to study and assess possible mechanisms.

BP 11.62 Tue 12:30 P1

Cumulative refractoriness in Calcium signaling — •Lukas Ramlow[1], Martin Falcke[1,2], and Benjamin Lindner[1] — [1]Physics Department of Humboldt University, Berlin, Germany — [2]Max Delbrück Center for Molecular Medicine, Berlin, Germany

Stochastic spiking and adaptation are two essential feature of calcium signaling. The stochasticty stems from the punctate calcium release from the ER into the cytosol by IP3R channel clusters. The adaptation is due to the depletion and slow replenishment of the ER. To capture calcium spike generation, we adopt the popular stochastic adaptive integral-and-fire (IF) model from neuroscience. Our model describes i) activity of IP3R clusters and ii) dynamics of the global calcium concentrations in the cytosol and ER. Cluster activity is modeled by a Markov chain, capturing the puff. The calcium concentrations are described by a two-variable IF model driven by the puff current. While it has been known for decades that the activity of IP3R clusters is random, a method to derive the noise acting on the cytosolic calcium is lacking. We close this gap using a time scale separation to approximate the puffing current by a white Gaussian noise with analytically accessible intensity. This results in a nonlinear IF model with and multiplicative noise. Assuming fast replenishment the IF model generates a renewal spike train and we can derive analytical expressions for the mean and coefficient of variation of the interspike interval (ISI).

Taking into account ER depletion, the model displays cumulative refractoriness and can be used to infer otherwise inaccesible parameters from experimental data.

BP 11.63 Tue 12:30 P1

Protein induced lipid demixing in homogeneous membranes — •Piotr Nowakowski[1,2], Bernd Henning Stumpf[3], Ana-Sunčana Smith[1,3], and Anna Maciołek[2,4] — [1]Institut Ruđer Bošković, Zagreb, Croatia — [2]Max Planck Institute for Intelligent Systems, Stuttgart, Germany — [3]Friedrich–Alexander–Universität Erlangen–Nürnberg, Erlangen, Germany — [4]Instytut Chemii Fizycznej Polskiej Akademii Nauk, Warszawa, Poland

We study a model of a lipid bilayer membrane with two order parameters: the chemical composition described using the Gaussian model and the spatial configuration described with the elastic deformation model of a membrane with a finite thickness, or equivalently, for an adherent membrane. We assume a linear coupling between the two order parameters. Using the exact solution, we calculate the correlation functions and order parameters profiles. We also study the domains that form around inclusions on the membrane. We propose and compare several distinct ways to quantify the size of such domains. Despite of its simplicity, the model has many interesting features like Fisher–Widom line and two distinct critical regions.

BP 11.64 Tue 12:30 P1

Self-organized criticality in animal collectives — •Yunus Sevinchan[1,2], David Bierbach[1,3,4], Luis Gómez-Nava[1,2], Jens Krause[1,3,4], and Pawel Romanczuk[1,2] — [1]Science of Intelligence, TU Berlin, Berlin, Germany — [2]Institute for Theoretical Biology, HU Berlin, Berlin, Germany — [3]Leibniz-Institute of Freshwater Ecology and Inland Fisheries, Berlin, Germany — [4]Thaer-Institute, HU Berlin, Berlin, Germany

Collective biological systems – such as animal groups or neuronal networks – are presumed to operate at or near so-called critical points at which they exhibit maximal sensitivity towards environmental cues. We have studied large fish shoals of sulphur mollies (*Poecilia sulphuraria*) which perform collective diving cascades as a response to predation. We previously found these shoals to operate close to criticality, allowing near-optimal propagation of information through the collective [1]. By analyzing a large video dataset of surface waves originating as a response to bird attacks or various synthetic stimuli, we relate wave characteristics to the macroscopic state of the shoal and varying environmental contexts. These results help in better understanding the fundamental mechanisms allowing collectives to self-tune their distance to criticality and navigate the robustness-sensitivity tradeoff.

[1]: L. Gómez-Nava, RT. Lange, PP. Klamser, J. Lukas, L. Arias-Rodriguez, D. Bierbach, J. Krause, H. Sprekeler, and P. Romanczuk: *Fish shoals maximize sensitivity towards external cues and show optimal information spread at criticality.* Nature Physics (accepted), **2022**

BP 11.65 Tue 12:30 P1

Electro-thermodynamics of coacervate interfaces — •Arghya Majee[1], Christoph A. Weber[2], and Frank Jülicher[1,3,4] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Institute of Physics, University of Augsburg, Germany — [3]Center for Systems Biology Dresden, Germany — [4]Cluster of Excellence Physics of Life, TU Dresden, Germany

Biological condensates are assemblies of proteins and nucleic acid that provide biochemical compartments in the cell. Such condensates can form by coacervation since many condensate components are charged and condensate properties vary with salt concentration. While the thermodynamic description based on short ranged interactions is well established, a theory accounting for the role of electrostatic interactions in the presence of salt is lacking. Here, we propose an electro-thermodynamic theory of such systems taking into account the role of electrostatics. We find that two or even more charged layers can form at the interface, where charge neutrality is locally not obeyed. Depending on the values of parameters, such charge profiles and associated electrostatic potential profiles imply either reflection or attraction of single molecules diffusing across the interface. Such interface properties could also account for a varying tendency of droplets to fuse and be of relevance for chemical reactions inside biological condensates by selectively recruiting reacting components by charge.

BP 11.66 Tue 12:30 P1

Mean-field theory for fibrillar aggregation and nematic-isotropic phase separation — •Kafa Alameh[1,2] and Christoph Weber[1] — [1]Mesoscopic Physics of Life, Institute of Physics, Universitätsstr. 1, Augsburg, Germany — [2]Center for Systems Biology Dresden, Pfotenhauerstr. 108, 01307 Dresden, Germany

Cells use droplet-like compartments to spatially organize their interior into sub-compartments, known as membrane-less organelles. Such organelles are liquid condensates and provide distinct physical environments for chemical processes. Recently, it has been shown that various proteins with beta-sheet structures, such as FUS, are involved in protein aggregation diseases such as ALS and Alzheimer's. Moreover, FUS-rich condensates were shown to undergo aberrant "phase transition," leading to fibrillar, solid-like aggregates. Several theoretical studies have focused on how phase-separated compartments affect the irreversible aggregation of dilute monomers; however, the interplay between aggregation and phase separation at non-dilute conditions remains elusive. Such conditions are particularly relevant at the condensate interface, where aggregates are often nucleated and enriched. Here, we propose a mean-field theory accounting for the interplay between aggregation, condensate formation, and phase transition at condensate interfaces. We find a rich phase behavior; three coexisting phases differing in density and the degree of order: disordered-dilute, disordered-dense, and nematic-dense phases. Our theory suggests the possibility of finding ordered membrane-less organelles in regulatory pathways of neurodegenerative diseases.

BP 11.67 Tue 12:30 P1

Density fluctuation analysis of living matter — •Conrad Möckel[1,2,3], Kyoohyun Kim[1,2], Abin Biswas[1,2,4], Simone Reber[4], Vasily Zaburdaev[1,2,5], and Jochen Guck[1,2,3] — [1]Max Planck Institute for the Science of Light, 91058 Erlangen, Germany — [2]Max Planck Zentrum für Physik und Medizin, 91058 Erlangen, Germany — [3]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91054 Erlangen, Germany — [4]IRI Life Sciences, Humboldt-Universität zu Berlin, 10115 Berlin, Germany — [5]Department of Biology, Mathematics in Life Sciences, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91054 Erlangen, Germany

The characterisation of the dynamical properties of living matter plays an important role in unraveling its complexity. Here we present the combination of quantitative phase imaging with differential dynamic microscopy in order to probe and evaluate its inherent density fluctuations. By employing theoretical models, this approach allows for the determination of the time- and length scale dependent viscoelastic properties of optically transparent systems as demonstrated for high speed supernatant (HSS) Xenopus laevis egg extract. We find that HSS exhibits distinct dynamics at two time scales which can be explained by diffusion in a diffusing potential.

BP 11.68 Tue 12:30 P1

Optimal navigation of smart active particles in complex landscapes — •Mischa Putzke and Holger Stark — Technische Universität Berlin, Institut für Theoretische Physik, Straße des 17. Juni 135, 10623 Berlin, Germany

The field of active matter, and in particular microswimmers, is finding more and more applications. Synthetic microswimmers are potentially used for microsurgery and the targeted transport of drugs and genes. This requires smart active particles that can process information.

The mentioned applications require the optimal navigation in complex environments where the self-propelled microswimmer only changes its orientation but not its velocity. Machine learning is often used to solve optimization problems. We employ Q-learning to train the agent to move towards a target while it receives information about the direction and distance of the target. To model the smart active particle we use Langevin dynamics.

We show that the microswimmer with its limited information is able to navigate in complex landscapes such as potential barriers and wells but also in vortical flow and find the fastest trajectories. We also show that the navigation optimization is stable against thermal fluctuations by including thermal noise in the orientation during training. For potential wells and vortical flow, it can also be observed that during training not the entire set of existing trajectories is covered by the microswimmer, thus optimal solutions can remain hidden.

BP 11.69 Tue 12:30 P1

Evaluation of nanoparticle resistance development of microorganisms — •Stefanie Schuba, Julian Schütt, Jürgen Fassbender, and Denys Makarov — Helmholtz-Zentrum Dresden-Rossendorf

Over the last century, antibiotics against bacterial infections have led to increased life expectancy and quality of people worldwide. Yet the WHO has brought attention to the increasing resistance development of bacterial pathogens against antibiotics - many bacteria are already multi-resistant. In the search of alternatives to classical antibiotics, nanotechnology and nanoparticles (NP) are moving into the focus of scientific research. Particular attention is paid to the Nano-silver (Ag-NP), which has experienced an immense upswing in recent years and is used in many medical products such as wound dressings or consumer products. However, are Ag-NPs safe for health and environment? To tackle this challenge, conventional methods have been used to explore nanoparticle resistance. Conversely, these methods have proven to be limited in terms of labor, cost, and statistical power. In our work, we intend to overcome these barriers by developing a droplet-based microfluidic analytical platform as a tool to elucidate the impact and biological influence of nanoparticles on living microorganisms with high statistical evaluation and detection efficiency. This method allows the separation of bacteria into single droplets, the generation of individual bioreactors, and the screening of the bacterial metabolism in the presence of Ag-NP.

BP 11.70 Tue 12:30 P1

Traffic Slowdown by Antibiotics — •Johannes Keisers, Luca Ciandrini, and Phillippe Fuchs — Centre De Structurale Biologe (CBS), Montpellier, France

The transcription and translation process are amongst the most fundamental processes in biology. In both processes, the flow of RNAP or ribosomes determines the biosynthesis rate. Here, we model this flow with a unidimensional traffic model called the Totally Asymmetric Simple Exclusion Process or TASEP. In particular, we are interested in understanding the role of ribosome pausing states induced by sublethal doses of antibiotics. These pausing states give furhter insights in the dynamics between different antibiotics and the translation process. The final goal is to model how antibiotics change the translation rate by adding a pausing state to the ribosomes and extend the previously derived solution to the open boundary case.

BP 11.71 Tue 12:30 P1

The Influence of pegRNA Variations on Prime Editing Kinetics — •Nathalie Schäffler[1], Julian Geilenkeuser[2], Dong-Jiunn Jeffery Truong[2], Gil Westmeyer[2], and Joachim Rädler[1] — [1]LMU München, Deutschland — [2]ISBM, Helmholtz-Zentrum München, Deutschland

A key development in recent CRISPR technology is the "Search and Replace" system, also called Prime Editing (PE). Right now, the optimization of this is an active research field, which could lead to interesting new possibilities like approaches for biocomputing. However, current studies focus primarily on endpoint measurements with FACS.

In our research we compare different pegRNA variations and their editing efficiency via collective and single cell timelapse measurements. We transfect a HEK293T cell line, which stably expresses a blue shifted mGreenLantern (bs-mGL), with the two PE components: pegRNA and Cas9-complex. With this, the cells gain the ability to edit their bsmGL DNA back to the original green mGL sequence. We track the fluorescence-time courses of this signal with Live-cell Imaging of Single Cell Arrays (LISCA) and use kinetic rate equations to better understand the defining processes in the timing of those edits.

This allows us to have a closer look into the kinetics of PE.

BP 11.72 Tue 12:30 P1

Steady-state operation of a cell-free genetic band-detection circuit — •Anna C. Jäkel, Lukas Aufinger, and Friedrich C. Simmel — Technichal University of Munich, Munich, Germany

Synthetic gene networks have been used extensively to explore principles of biological pattern formation as they play a decisive role during biological growth and development processes. Here, we report on a bottom-up approach to design and analyze a cell-free genetic circuit based on an incoherent feed forward loop (IFFL-2), which is expected to produce a three-stripe pattern in response to an input gradient. In our work, we first simulated the behavior of the circuit and explored relevant parameters using a genetic algorithm. We then tested our circuit in a bacterial cell-free gene expression system and found that our circuit is only functional under non-equilibrium conditions in microfluidic ring reactors, whereas it fails to perform in bulk experiments in closed reactors. Hence, we concluded that non-equilibrium conditions are of necessity to establish the double-repression cascade which was the essential element of the genetic circuit. We used six neighboring ring reactors to establish a 'virtual' morphogen gradient by supplying the reactors with decreasing amounts of the transcription factor sigma28, corresponding to the different positions within an exponential morphogen gradient. We finally demonstrated that our IFFL-2 circuit, when operated in the microfluidic system, shows the correct gene expression response that is required for stripe-formation in a spatial context.

BP 11.73 Tue 12:30 P1

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BP 11.74 Tue 12:30 P1

A first approach for mimicking guided axon-growth by electrical circuits — •Bakr Al Beattie, Sebastian Jenderny, Karlheinz Ochs, and Dennis Michaelis — Ruhr University Bochum, Chair of Digital Communication Systems, Bochum, Germany

The self-organization aspect of electrical circuits mimicking neuronal networks often only focuses on synapses. Besides the adjustment of synaptic coupling strength, the guidance of growing axons is another important principle for the biological wiring process of neurons. In particular, guidance cues determine the growth direction and thus which neurons interconnect with each other. Up to now, only mathematical models of this process exist. Our aim hence is to provide an ideal electrical circuit mimicking fundamental principles of guided axon growth. For this purpose, we use memristors in combination with sensors. Here, the sensors represent the sensing of guidance cues, while the memristors form the non-volatile signal transmission paths. We then develop a corresponding wave digital model to verify our circuit approach.

BP 11.75 Tue 12:30 P1

Mimicking axon-growth by a bio-inspired memristive circuit — Sebastian Jenderny, •Bakr Al Beattie, and Karlheinz Ochs — Ruhr University Bochum, Chair of Digital Communication Systems, Bochum, Germany

Hardware implementations of neuronal networks are already very powerful. In terms of e.g. energy efficiency, however, they are still far inferior to biological neuronal networks. For this purpose, a better understanding of the general principles that shape these networks can contribute to the development of improved electrical circuits. One principle often neglected is the growing of axons, which has, up to now, only been considered for technical abstract circuit realizations. In this context, our aim is to develop a more bio-inspired circuit model mimicking axon growth in a way that can be compared to the biological process. To this end, we utilize Morris-Lecar oscillators as axon segments and memristors for implementing the growth mechanism. A wave digital emulation then successfully verifies our circuit approach for an axon growth example taken from biology.

BP 11.76 Tue 12:30 P1

RNA Contact Prediction by Data Efficient Deep Learning — •Oskar Taubert[1], Fabrice Lehr[2], Alina Bazarova[3,4], Christian Faber[3], Philipp Knechtges[2], Marie Weiel[1,4], Charlotte Debus[1,4], Daniel Coquelin[1,4], Achim Basermann[2], Achim Streit[1], Stefan Kesselheim[3,4], Markus Götz[1,4], and Alexander

Schug[3] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Deutsches Zentrum für Luft- und Raumfahrt, Köln, Germany — [3]Forschungszentrum Jülich, Jülich, Germany — [4]Helmholtz AI

On the path to full understanding of the structure-function relationship or even design of RNA, structure prediction would offer an intriguing complement to experimental efforts. Any deep learning on RNA structure, however, is hampered by the sparsity of labeled training data. Utilizing the limited data available, we here focus on predicting spatial adjacencies (*contact maps*) as a proxy for 3D structure. We explore the space of self-supervised learning for RNA multiple sequence alignments and focus on downstream contact prediction from latent attention maps.

Boosted decision trees in particular prove an advancement in contact prediction quality that can be further enhanced by finetuning the pretrained backbone. We name our model BARNACLE. Our conceptional advance is reflected by a considerable increase of precision and other metrics for contact prediction, thus promising to decrease the sequence-structure gap for RNA.

BP 11.77 Tue 12:30 P1

Influence of Contact Map Topology on RNA Structure Prediction — •Christian Faber and Alexander Schug — Forschungszentrum Jülich, Germany

The available sequence data of RNA molecules have highly increased in the past years. Unfortunately, while computational power is still under exponential growth, the computer prediction quality from sequence to final structure is still inferior to the labour intensive experimental work. Therefore, various attempts have been made to improve computer generated structure predictions.

Although an end-to-end procedure has been developed for proteins in the form of Alphafold2, such a breakthrough is not yet available for RNA molecules. The current strategy entails two steps: (i) predicting potential contacts in the form of a contact maps from evolutionary data, and (ii) simulating the molecule with a physical force field while using the contact map as restraint. However, the quality of the structure prediction crucially depends on the quality of the contact map.

Until now, only the proportion of true positive contacts was considered as a quality characteristic. We propose to also include the distribution of these contacts, and have done so in our recent studies. We observed that the distribution into clusters (typical for ML) leads to poor results. Therefore, we propose a new quality criterion for contact maps that can be easily incorporated into existing ML algorithms. We have introduced this criterion into Barnacle, a recent, very strong ML algorithm especially designed for RNA contact prediction.

BP 11.78 Tue 12:30 P1

Combined cell and nanoparticle models for TOPAS to study radiation dose enhancement by Monte-Carlo based particle scattering Simulations — •Marc Benjamin Hahn[1] and Julian Mateo Zutta Villate[2] — [1]Bundesanstalt für Materialforschung und -prüfung, 12205 Berlin, Germany — [2]Pontificia Universidad Javeriana, Bogota, Colombia

Dose enhancement by gold nanoparticles (AuNP) increases the biological effectiveness of radiation damage in biomolecules and tissue. To apply them effectively during cancer therapy their influence on the locally delivered dose has to be determined.[1] Hereby, the AuNP locations strongly influence the energy deposit in the nucleus, mitochondria, membrane and the cytosol of the targeted cells. In this work, two newly developed continuous and discrete-geometric models for simulations of AuNP in cells are presented.[2] We apply the presented models in Monte-Carlo particle scattering simulations to characterize the energy deposit in cell organelles by radioactive 198AuNP. They emit beta and gamma rays and are therefore considered for applications with solid tumors. Differences in local dose enhancement between randomly distributed and nucleus targeted nanoparticles are compared. Hereby nucleus targeted nanoparticels showed a strong local dose enhancement in the radio sensitive nucleus.[1] J.M. Zutta Villate and M.B. Hahn, Eur. Phys. J. D. 73 (2019) 95. [2] M.B. Hahn and J.M. Zutta Villate, Sci Rep 11 (2021) 6721.

BP 12: Biopolymers and Biomaterials (joint session BP/CPP)

Time: Wednesday 9:30–13:00 Location: TOE 317

BP 12.1 Wed 9:30 TOE 317

Interaction of laminin and brain cells with ion implanted titania nanotube scaffolds — •Jan Frenzel[1,2,3], Astrid Kupferer[1,2], and Stefan Mayr[1,2] — [1]Leibniz Institute of Surface Engineering (IOM), 04318 Leipzig, Germany — [2]Division of Surface Physics, Faculty of Physics and Earth Sciences, Leipzig University, 04103 Leipzig, Germanyany — [3]Research Group Biotechnology and Biomedicine, Faculty of Physics and Earth Sciences, Leipzig University, 04103 Leipzig, Germany

Brain-machine interfaces enable symptomatic treatment of neurodegenerative diseases by modulating neural activities and enjoy great popularity when brain tissue is assessed ex vivo. However, current-use interface materials are troubled by numerous challenges concerning loss of long-term adhesion, rejection reactions, and glial scarring. We show that ion-implanted titania nanotube scaffolds (TNS) are a promising candidate for dealing with these issues because they combine high biocompatibility with adequate electrical conductivity. Based on our experiments, we explain how changes in the adsorption of laminin and the viability/adhesion of neurons and glial cells caused by ion implantation can be described by alterations in surface characterisics. The high neuron viability observed on all TNS, but suppressed glial cell formation on implanted TNS, demonstrates the potential as a future interface material. We acknowledge funding by SMWK (100331694). Reference: Frenzel et al., Nanomaterials 2022, 12, 3858. https://doi.org/10.3390/nano12213858

BP 12.2 Wed 9:45 TOE 317

Fiber-based femtosecond 3D printing — •Claudia Imiolczyk[1], Andy Steinmann[1], Moritz Flöss[1], Zhen Wang[1], Michael Heymann[2], Andrea Toulouse[3], and Harald Giessen[1] — [1]4th Physics Institute, Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Institute of Biomaterials and Biomolecular Systems, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [3]Institute of Applied Optics, Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart, Germany

Ultrashort laser pulses are often used in medical applications, for instance for soft-tissue surgeries. However, the progress on using such laser pulses for tissue structuring is rather marginal so far. Therefore, we aim to realize an endoscopic fiber-based femtosecond 3D printer to minimally invasively surgically repair organ damage on a micrometer scale. For this, high-power femtosecond laser pulses are required, in order to 3D print desired geometries with a microfluidic bio-ink using two-photon-lithography. We utilize ruled reflective diffraction gratings to pre-chirp laser pulses, as dispersion in optical fibers broadens these femtosecond laser pulses. We report on measurements of pulse duration, spectrum, compression, and nonlinear effects. These resulting 3D printed structures should be colonized with endogenous cells, analogous to the extracellular matrix. This could open a new area of endoscopic 3D printing of biomaterials inside the human body to revolutionize plastic micro-surgery, such as repairing defects in the heart of embryos or even repairs behind the eardrum at the auditory ossicles.

BP 12.3 Wed 10:00 TOE 317

DNA-encoded viscoelastic matrices for cell and organoid culture — •Elisha Krieg — Leibniz-Institut für Polymerforschung Dresden e.V. — Technische Universität Dresden

The recent advances in mechanobiology and the physics of life have driven an immense interest in mechanically programmable viscoelastic materials for cell and organoid culture. Here I describe a class of soft hydrogels based on novel DNA libraries that self-assemble with synthetic polymers.[1] This dynamic DNA-based matrix (DyNAtrix) provides computationally predictable, systematic, and independent control over key cell-instructive properties by merely changing DNA sequence information without affecting the compositional features of the system. This approach enables: (1) thermodynamic and kinetic control over network formation; (2) adjustable heat activation for the homogeneous embedding of mammalian cells; and (3) dynamic tuning of stress relaxation times to precisely recapitulate the mechanical charac-

teristics of living tissues. DyNAtrix is self-healing, printable, exhibits high stability, cyto- and hemocompatibility, and controllable degradation. DyNAtrix-based 3D cultures of human mesenchymal stromal cells, pluripotent stem cells, canine kidney cysts, and placental organoids exhibit high viability, proliferation, and morphogenesis over several days to weeks. DyNAtrix thus represents a programmable and versatile precision matrix, paving the way for advanced approaches to biomechanics, biophysics, and tissue engineering.

[1] Peng et al. bioRxiv 2022, DOI:10.1101/2022.10.08.510936

Invited Talk BP 12.4 Wed 10:15 TOE 317

Materials properties of bacterial biofilms. — •Cécile M. Bidan — Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Potsdam, Germany

As bio-sourced materials are raising interest for their sustainability, using bacteria to produce biofilms made of a protein and polysaccharide matrix has become a new strategy to make engineered living materials with various functionalities. Our group contributes to this emerging field by clarifying how bacteria adapt biofilm materials properties to the environment. For this, we culture E. coli producing curli amyloid and phosphoethanolamine-cellulose fibers on nutritive agar substrates with varying physico-chemical properties and study the growth, morphology and mechanical properties of the resulting biofilms. We demonstrated that changing the properties of the agar substrate with polyelectrolyte coatings or by varying the water content the bulk properties of the agar affects E. coli biofilm growth, morphology and mechanical properties. We also used E. coli producing only amyloid fibers and focus on the matrix structural and functional changes at the molecular scale. To assess the contribution of each matrix component to the macroscopic biofilm materials properties, we compared the characteristics of biofilms produced by a collection of E. coli mutants differing in the matrix they produce. The results indicate that E. coli biofilm matrix is a composite made of rigid and brittle curli amyloid fibers assembled within a mesh of soft and adhesive phosphoethanolamine-cellulose fibers. Finally, we explored how treating biofilms with ionic solutions can help tuning further their properties.

BP 12.5 Wed 10:45 TOE 317

The migration and search behavior of immune cells — Reza Shaebani and •Franziska Lautenschläger — Saarland University, Saarbrücken

Immune cells have a variety of tasks in the body. For example, dendritic cells act as the *sentinels* searching for pathogens. For this search, the cells need to scan a certain area in an effective way. Here, we investigate how cells optimize the search of such area. We have shown before that all cell types show a correlation of migration speed and persistence [1]. We later found that cells which strongly correlate these two parameters are particularly good at searching objects [2]. Interestingly, we found that cells do not keep the memory of their speed as long as the memory of their persistence [3]. Now, we investigate how we can disturb this migration and search behavior, preferable by altering the cytoskeleton [4].

1.*Maiuri, P., et al., Actin flows mediate a universal coupling between cell speed and cell persistence. Cell, 2015. 161(2): p. 374-86. 2.*Shaebani, M.R., et al., Persistence-Speed Coupling Enhances the Search Efficiency of Migrating Immune Cells. Phys Rev Lett, 2020. 125(26): p. 268102. 3.*Shaebani, M.R., M. Piel, and F. Lautenschläger, Distinct Speed and Direction Memories of Migrating Cells Diversify Their Possible Search Strategies. arXiv. 4.*Shaebani, M.R., et al., Vimentin provides target search efficiency and mechanical resilience for dendritic cell migration. bioRxiv, 2020: p. 2020.12.18.423401.

BP 12.6 Wed 11:00 TOE 317

Molecular motors from a 3D perspective: how do kinesins organize microtubules? — •Laura Meissner[1], Jonas Bosche[2], Ludger Santen[2], and Stefan Diez[1,3,4] — [1]B CUBE - Center for Molecular Bioengineering, TU Dresden, Dresden, Germany — [2]Center for Biophysics, Department of Physics, Saarland University, Saarbrücken, Germany — [3]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany — [4]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Kinesins are ubiquitous motor proteins that are essential for intracellular transport processes. In addition, several kinesins act within the mitotic spindle by sliding and crosslinking microtubules. Some of those kinesins not only move longitudinally on the microtubule filament but also display an axial component in their motion. So far, the effect of this axial motion on motility and force generation within the mitotic spindle has not been explored deeply. Using a 3D motility assay, we show that the antagonistic motor proteins kinesin-5 and kinesin-14 drive the rotation of microtubules around each other. We characterize their motility parameters, including velocity and pitch. Further, we determine the extension of the motors, which reveals the conformation of the motors in microtubule overlaps. To investigate the rotational force (torque) that the motors could produce during microtubule sliding, we developed a microtubule coiling assay. Here, both kinesin-5 and kinesin-14 bent and coiled microtubules, indicative of the generation of significant torque. We hypothesize that this behavior serves to organize spindle fibers and to provide robustness to the spindle.

15 min. break

BP 12.7 Wed 11:30 TOE 317

3D stimulated Raman spectral imaging of water dynamics associated with pectin-glycocalyceal entanglement — •Moritz Floess[1], Tobias Steinle[1], Florian Werner[1], Yunshan Wang[1], Willi L. Wagner[2], Verena Steinle[2], Betty S. Liu[3], Yifan Zheng[3], Steven J. Mentzer[3], and Harald Giessen[1] — [1]4th Physics Institute, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Department of Diagnostic and Interventional Radiology, University Hospital of Heidelberg, Im Neuenheimer Feld 420, 69120 Heidelberg, Germany — [3]Laboratory of Adaptive and Regenerative Biology, Brigham & Women's Hospital, Harvard Medical School, Boston MA

Pectin, a heteropolysaccharide, is an ideal biomaterial for medical applications such as serosal wound healing and visceral tissue repair. It forms strong mechanical bonds with the underlying tissue. The extraordinary adhesive properties of pectin on organ surfaces are highly water-dependent and most likely result from a microstructural entanglement of pectin polysaccharide chains with the similarly textured glycocalyx, a glycoprotein coat, covering mammalian cell surfaces. We employ label-free 3D stimulated Raman scattering (SRS) microscopy to investigate the hydrophilicity of pectin hydrogel without the altering effects of sample fixation, dehydration, or tissue staining. In particular, we quantify the time scales, on which two different hydration mechanisms take place. Furthermore, the transition zone between pectin and porcine serosal tissue is imaged to obtain quantitative insights into the entanglement between pectin and mammalian glycocalyx.

BP 12.8 Wed 11:45 TOE 317

Quantifying optomechanical properties of phase separated protein condensates — •Timon Beck[1], Lize van der Linden[2], Raimund Schlüssler[2], Kyoohyun Kim[1], Simon Alberti[2], and Jochen Guck[1] — [1]Max Planck Institute for the Science of Light, Erlangen, Germany — [2]Biotec TU Dresden, Dresden, Germany

The organization of intracellular material is a complex task and cells have different strategies for compartmentalization. One way is the formation of membraneless organelles that are involved, for example, in metabolic control and DNA repair. The underlying process of phase separation and percolation is tightly controlled by many parameters as temperature, ion and protein concentration, as well as crowding conditions. Changes in these parameters have an impact on the intermolecular interactions and accordingly tune optical and viscoelastic characteristics of the condensates. Despite the dynamic development of the research field in the last years, there is a lack of tools to quantitatively measure such physical properties. A combination of Brillouin microscopy with quantitative phase imaging, providing information about refractive index and density, gives access to a set of optical and mechanical quantities and in particular the longitudinal modulus. By varying temperature and ion conditions, we were able to tune intermolecular interactions within phase separated protein droplets and found that the introduced variations are reflected in the optomechanical properties of the condensates.

BP 12.9 Wed 12:00 TOE 317

Confinement-induced fractionation and liquid-liquid phase separation of polymer mixtures — •Arash Nikoubashman[1] and Miho Yanagisawa[2] — [1]Institute of Physics, JGU Mainz, Germany — [2]Graduate School of Science, The University of Tokyo, Japan

The formation of (bio)molecular condensates via liquid-liquid phase separation in cells has received increasing attention, as these coacervates play important functional and regulatory roles within biological systems. However, the majority of studies focused on the behavior of pure systems in bulk solutions, thus neglecting confinement effects

and the interplay between the numerous molecules present in cells. To advance our knowledge, we perform simulations of binary polymer mixtures in droplets, considering both monodisperse and polydisperse molecular weight distributions for the longer polymer species. We find that confinement induces a spatial separation of the polymers by length, with the shorter ones moving to the droplet surface. This partitioning causes a distinct increase of the local polymer concentration in the droplet center, which is more pronounced in polydisperse systems. Consequently, the systems exhibit liquid-liquid phase separation at average polymer concentrations where bulk systems are still in the one-phase regime.

BP 12.10 Wed 12:15 TOE 317

Branching morphogenesis in the silica cell wall of diatoms — •Iaroslav Babenko[1,2,3], Benjamin M. Friedrich[1,2], and Nils Kröger[1,3] — [1]Cluster of Excellence Physics of Life, TU Dresden, 01062 Dresden, Germany. — [2]Center of Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany. — [3]Center for Molecular and Cellular Bioengineering, 01307 Dresden, Germany.

Diatoms live in a glass house: these common single-celled algae fascinated evolutionary biologists, chemical engineers and inspired artists for their ability to produce intricately nano- and micropatterned silica schells. The valve of the cell wall is formed in a planar intracellular compartment termed silica deposition vesicles (SDVs). The physical mechanism that guides the self-assembly of species-specific silica patterns is unknown. Here, we address this question by studying the formation of the silica rib patterns in the cell wall of the model diatom *Thalassiosira pseudonana* by combining theory and electron microscopy of nascent silica valves. We propose a minimal model of branching morphogenesis based on a non classical Turing reaction-diffusion system to quantitatively account for the time course of experimentally observed rib patterns. We introduce a novel mechanism of branching morphogenesis, which relies on a transition from soluble to insoluble silica phases inside the SDV and the concurrent release of an inhibitor that hinders this transition. Moreover, our minimal model is capable of producing a wide range of rib patterns, suggesting that this model may be applicable for describing branching morphogenesis in other diatom species and potentially, in other organisms.

BP 12.11 Wed 12:30 TOE 317

Reimplementing the formation and dispersal of transcriptional clusters with synthetic DNA-nanomotifs and Langevin-dynamics simulations — •Aaron Gadzekpo[1], Xenia Tschurikow[1], Mai Tran[2], Rakesh Chatterjee[3,4], Vasily Zaburdaev[3,4], Kerstin Göpfrich[2], and Lennart Hilbert[1] — [1]Karlsruhe Institute of Technology — [2]Max Planck Institute for Medical Research — [3]Max Planck Zentrum für Physik und Medizin — [4]Friedrich-Alexander Universität Erlangen-Nürnberg

Spatial organisation of the genome is emerging as a crucial aspect of gene transcription. In pluripotent cells, self-interacting molecular factors, such as RNA polymerase II, form microphase-separated domains, which become increasingly dispersed due to amphiphilic effects of newly transcribed genes. To understand the principles that lead to this behaviour, we designed synthetic DNA-nanomotifs that form droplets due to self-interaction and allow for the addition of an amphiphilic tail of thymines. Time-lapse microscopy, titration experiments and analysis of the resulting distributions of droplet properties demonstrate that the synthetic system reproduces the dispersal of phase-separated domains found for increasing transcription levels. Simulations based on Langevin-dynamics equally reproduce this behaviour after tuning interaction strengths and number ratios. Our findings illustrate how model-guided design of DNA-based systems can elucidate the mechanisms that control spatio-temporal compartmentalisation in cells.

BP 12.12 Wed 12:45 TOE 317

Partition complex structure can arise from sliding and bridging of ParB dimers — •Lara Connolley[1], Lucas Schnabel[2], Martin Thanbichler[2], and Sean Murray[1] — [1]Max Planck Institute for Terrestrial Microbiology, Marburg, Germany — [2]University of Marburg, Marburg, Germany

Chromosome segregation is vital for cell replication and in many bacteria is controlled by the ParABS system. A key part of this machinery is the association of ParB proteins to the parS-containing centromeric region to form the partition complex. Despite much work, the formation and structure of this nucleoprotein complex has remained unclear. It was recently discovered that CTP binding allows ParB dimers to entrap and slide along the DNA, as well as leading to more efficient condensation through ParB-mediated DNA bridging. Here, we use semi-flexible polymer simulations to show how these properties of sliding and bridging can explain partition complex formation. We find that transient ParB bridges can organise the DNA into either a globular state or into hairpins and helical structures, depending on the bridge lifetime. Upon coupling with stochastic sliding simulations to form a unified sliding and bridging model, we find that short-lived ParB bridges do not hinder ParB sliding and the model can reproduce both the ParB binding profile and the condensation of the nucleoprotein complex. Overall, our model clarifies the mechanism of partition complex formation and predicts its fine structure.

BP 13: Signaling, Biological Networks

Time: Wednesday 9:30–11:00 Location: BAR 0106

Invited Talk BP 13.1 Wed 9:30 BAR 0106

Biological signal processes across scales — •Steffen Rulands — Ludwig-Maximilians Universität München, Arnold Sommerfeld Center ffor theoretical Physics, Theresienstr. 37, 80333 München — Max-Planck-Institute for theoretical Physics, Nöthnitzer Str. 38, 01187 Dresden

In contrast to many physical systems, biological systems have the remarkable architecture of being organized into a spatial hierarchy of non-equilibrium processes: from molecules embedded into sub-cellular compartments to cells interacting in tissues. In my talk, I will show how biological systems manipulate the transmission of noise and information between and across these scales in order to perform biological functions. By combining theory and experiments I will first describe a general theory describing the propagation of noise and signals in multi-scale non-equilibrium systems. I will then apply these insights to show how cells make use of the propagation of fluctuations on the subcellular scale to perform biological signal processing: by establishing a low-pass filter of concentration fluctuations in the regulation of cell death and by facilitating a gelation phase transition in the innate immune response.

BP 13.2 Wed 10:00 BAR 0106

Protein Dynamics in the Complex Physical Environment of the Synapse — •Simon Dannenberg, Sarah Mohammadinejad, and Stefan Klumpp — Institut für Dynamik komplexer Systeme Georg-August-Universität Göttingen, Göttingen, Germany

The synapse is a complex environment that is densely packed with proteins and has an internal geometry structured by membranes. This affects the mobility of proteins involved in signal transmission and hence, their availability at corresponding reaction sides.

In our work we use dynamic Monte Carlo simulations to investigate the influence of different physical features of the synapse on protein mobility. The simulations are parameterized by mobility measurements via FRAP experiments. Our approach revealed an unexpectedly high sensitivity of the experiments on the geometry of the synapses as well as dependence of protein fluxes on synaptic features such as axon diameter and synapse size.

BP 13.3 Wed 10:15 BAR 0106

How can a single neuron influence behavior? Hints from integrate-and-fire network models — •Davide Bernardi[1] and Benjamin Lindner[2,3] — [1]Italian Institute of Technology, Ferrara, Italy — [2]Bernstein Center for Computational Neuroscience, Berlin, Germany — [3]Institut für Physik, Humboldt-Universität zu Berlin

Recent experiments challenge the established view that only large neuronal populations can reliably encode information, as is argued on the basis of the large noise and chaotic dynamics of cortical networks. One striking example is that awake rats can be trained to respond to the stimulation of a single cell in the barrel cortex. Here, this problem is framed theoretically by studying how the stimulation of a single neuron

can be detected in large networks of integrate-and-fire neurons.

Combining numerical simulations and analytical calculations, we illustrate a simple strategy to detect the single neuron stimulation in the activity of a readout subpopulation or in a second network, which is both more realistic and more efficient. Furthermore, a readout network tuned to approximate a differentiator circuit can detect the single-neuron stimulation in a more biologically detailed model. In this case, the detection probability increases significantly upon injection of an irregular current, in agreement with experiments.

Our models show how inhibitory synapses could make it possible for the sensitivity to single-neuron perturbation to coexist with a stable asynchronous spontaneous activity, that is, through a mild selective imbalance in the topological (spatial) and temporal sense.

BP 13.4 Wed 10:30 BAR 0106

Towards statistical models of activity recordings from stem cell derived neuronal networks — •Sebastian Willenberg[1], Elijah R. Shelton[1], Paulina M. Wysmolek[2], Filippo D. Kiessler[1], Achim Brinkop[1], and Friedhelm Serwane[1,2,3] — [1]Faculty of Physics and CeNS, LMU, Munich, Germany — [2]MPI for Medical Research, Heidelberg, Germany — [3]Munich Cluster for Systems Neurology, Munich, Germany

Analysis of neuronal activity is the key to understanding the principles of brain circuitry. Theoretical models have been applied on many different scales, ranging from the analysis of single neuron activity to the collective behaviour of large groups of neurons. Models from statistical physics describe the behaviour of networks across spatial and temporal scales with a minimal amount of parameters. Until now, those models have mainly been applied to datasets recorded via 2D electrode arrays. This makes accessing 3D network morphology challenging. I will present our first steps applying statistical models to neuronal recordings of stem cell derived neuronal networks obtained using lightsheet or confocal microscopy. To model the collective firing we map single neuron activity to two states and apply a maximum entropy model to calculate the entropy and energy following the approach of Tkačik et al.[2]. Using this approach, we seek a minimal model describing the firing activity which allows us to understand and predict the collective behaviour of *in vitro* neuronal networks.

1: Wysmolek et al., Sci Rep 12, 20420, 2022
2: Tkačik et al., PNAS 112, 11508, 2015

BP 13.5 Wed 10:45 BAR 0106

Inference of dynamical networks connectivity with Recurrent Neural Networks — •Pablo Rojas, Marie Kempkes, and Martin E Garcia — Theoretical Physics, University of Kassel, Germany

The inference of directed links in networks of interacting systems is a problem spanning many disciplines. Systems out of equilibrium represent a special case, where samples are not independent but structured as timeseries. In this context, Recurrent Neural Networks (RNN) have attracted recent attention, due to their ability to learn dynamical systems from sequences. We introduce a method to infer connectivity of a network from the timeseries of its nodes, using a RNN based on Reservoir Computing (RC). We show how modifications of the standard RC architecture enable a reliable computation of the existence of links between nodes. While the method does not require information about the underlying mathematical model, its performance is further improved if the selection of hyperparameters is roughly informed by knowledge about the system. The method is illustrated with examples from different complex systems, ranging from networks of chaotic Lorenz attractors to biological neurons. Using simulations of these systems, we demonstrate its power and limitations under a variety of conditions, such as noise levels, delayed interactions, size of the network and hidden variables.

BP 14: Focus Session: From Inter-individual Variability to Heterogeneous Group Dynamics and Disorder in Active Matter (joint session DY/BP/CPP)

The study of active particle dynamics has developed into a vibrant field of multidisciplinary research, including such diverse systems as bacterial colonies, cellular self-organization, synthetic colloids and microrobots as well as macroscopic systems like locusts, flocks of birds, schools of fish or pedestrians. Whereas many studies in the past focused either on the random transport of individual particles or on the interplay of temporal fluctuations (noise) and interactions (velocity alignment or attraction/repulsion), there is now an increasing interest in the question how structural disorder and inter-individual variability, i.e., different motility characteristics of individuals, shape the active particle dynamics and emergent pattern formation of groups. The presence of structural or quenched disorder raises furthermore the immediate question how to bridge data and models based on (short time) tracking data, given the simultaneous presence of temporal fluctuations. With this focus session, we aim at bringing researchers from statistical physics and biophysics together to discuss this interdisciplinary topic and exchange ideas on common challenges arising in different application areas.

Organized by Robert Großmann (Potsdam)

Time: Wednesday 9:30–13:00 Location: ZEU 160

Invited Talk BP 14.1 Wed 9:30 ZEU 160

More is different: High-throughput 3D tracking reveals bacterial navigation strategies — •Katja Taute — Rowland Institute at Harvard, Harvard University, Cambridge, MA, USA — Department of Biology, Microbiology, LMU München, 82152 Martinsried, Germany

How microbes navigate environmental chemical gradients has implications that range from health to climate. The behavioral mechanisms underlying chemotaxis are unknown for most species because of a lack of techniques capable of bridging scales from individual navigation behavior to the resulting population-level performance. We present a multiscale 3D chemotaxis assay that combines high-throughput 3D bacterial tracking with microfluidically created chemical gradients. Large datasets of 3D trajectories yield the statistical power required to assess chemotactic performance at the population scale, while simultaneously resolving the underlying 3D navigation behavior for every individual. Applying this technique to the well-studied model bacterium Escherichia coli, we uncover dramatic, previously unknown heterogeneity in chemotactic performance. We investigate the underlying behavioral mechanisms and discuss potential implications at the population level.

Invited Talk BP 14.2 Wed 10:00 ZEU 160

Variability and heterogeneity in natural swarms — •Gil Ariel — Bar Ilan University, Ramat Gan, Israel

Collective motion of large-scale natural swarms, such as moving animal groups or expanding bacterial colonies, have been described as self-organized phenomena. Thus, it is clear that the observed macroscopic, coarse-grained swarm dynamics depend on the properties of the individuals of which it is composed. In nature, individuals are never identical, and may differ in practically every parameter. Hence, intra-group variability and its effect on the ability to form coordinated motion is of interest, both from theoretical and a biological points of view. In this talk, I will review and examine some of the fundamental properties of heterogeneous collectives in nature, with an emphasis on two widely-used model organisms - swarming bacteria and locusts. Theoretical attempts to explain the observed phenomena will be discussed in view of laboratory experiments, highlighting their successes

and failures. While heterogeneity typically discourages collectivity, there are several natural examples where it has an opposite effect.

BP 14.3 Wed 10:30 ZEU 160

Effect of individual differences on the jamming transition in traffic flow — •Yi-Chieh Lai and Kuo-An Wu — Department of Physics, National Tsing Hua University, 30013 Hsinchu, Taiwan

The individual difference, particularly in drivers' distance perception, is introduced in the microscopic one-dimensional optimal velocity model to investigate its effect on the onset of the jamming instability seen in traffic systems. We show analytically and numerically that the individual difference helps to inhibit the traffic jam at high vehicle densities while it promotes jamming transition at low vehicle densities. In addition, the jamming mechanism is further investigated by tracking how the spatial disturbance travels through traffics. We find that the jamming instability is uniquely determined by the overall distribution of drivers' distance perception rather than the spatial ordering of vehicles. Finally, a generalized form of the optimal velocity function is considered to show the universality of the effect of the individual difference.

BP 14.4 Wed 10:45 ZEU 160

Distinct impacts of polar and nematic self-propulsion on active unjamming — Varun Venkatesh[1], •Chandana Mondal[2], and Amin Doostmohammadi[1] — [1]Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, 2100 Copenhagen, Denmark — [2]UGC-DAE CSR, University Campus, Khandwa Road, Indore 452017, India

We explore, by MD simulations, the jamming-unjamming transition in a dense system of active semiflexible filaments. In particular, we characterize the distinct impact of polar vs nematic driving for different filament rigidities and at varying densities. Our results show that high densities of dynamic active filaments can be achieved by only changing the nature of the active force, nematic or polar. Interestingly, while polar driving is more effective at unjamming the system at high densities below confluency, we find that at even higher densities, nematic driving enhances unjamming compared to its polar counterpart. The effect of varying the rigidity of filaments is also significantly different in the two cases: While for nematic driving, lowering the bending rigidity unjams the system, we find an intriguing reentrant jamming-unjamming-jamming transition for polar driving as the filament rigidity is lowered. While the first transition (unjamming) is driven by softening due to reduced rigidity, the second transition (jamming) is a cooperative effect of ordering and coincides with the emergence of nematic order in the system. Together, through a generic model of self-propelled flexible filaments, our results demonstrate how tuning the nature of self-propulsion and flexibility can be employed by active materials to achieve high densities without getting jammed.

15 min. break

Invited Talk BP 14.5 Wed 11:15 ZEU 160

Superstatistical Analysis and Modelling of Complex Dynamical Systems — •Claus Metzner[1,2], Christoph Mark[2], Ben Fabry[2], Patrick Krauss[1], Achim Schilling[1], Maximilian Traxdorf[3], and Holger Schulze[1] — [1]Neuroscience Lab, University Hospital Erlangen, Germany — [2]Biophysics Lab, Friedrich-Alexander Universität Erlangen-Nürnberg — [3]Department of Otorhinolaryngology, Head and Neck Surgery, Paracelsus Medical University, Nuremberg, Germany

On longer time scales, complex systems often pass through different dynamical attractors and thus produce 'anomalous' distributions and correlations when analyzed with conventional statistical tools. We argue that the most appropriate way of describing such systems is by hierarchical multilevel models, in which the lowest level is a relatively simple random walk model that can generate the observed time series on short time scales, but which depends on latent hyper-parameters that are themselves time-dependent and controlled by the higher levels of the model. First, our Bayesian method is introduced for the sequential inference of those gradual or abrupt parameter changes. We then review possible applications of the superstatistical framework in such diverse fields as biophysics, neuroscience, finance, or policy assessment. Finally, we discuss more recent extensions of the method for model selection and the use of machine learning models for estimating complex likelihood functions.

BP 14.6 Wed 11:45 ZEU 160

How to infer parameter distributions in heterogeneous populations of active particles — •Jan Albrecht[1], Robert Grossmann[1], and Manfred Opper[2,3] — [1]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [2]TU Berlin, Fakultät IV-MAR 4-2, Marchstraße 23, 10587 Berlin, Germany — [3]Centre for Systems Modelling and Quantitative Biomedicine, University of Birmingham, B15 2TT, United Kingdom

Experiments with active particles, e.g., motile microorganisms like bacteria or amebae, provide information about their position at discrete points in time. However, most active particle models, like active Ornstein-Uhlenbeck particles for example, are commonly described by first order stochastic differential equations for the velocity or force. This leads to a second order model in position posing challenges for parameter inference, because there is no general way to obtain a closed form expression for the likelihood of the parameters in terms of those time-sampled trajectories. This would be needed to apply efficient Bayesian parameter estimation techniques. In this talk, we propose a filtering-like sequential method to address this problem. The likelihood is first expressed in terms of integrals over transition probabilities. Approximating the transition probability for small times makes these integrals analytically feasible, leading to a likelihood approximation that allows consistent parameter inference. Using a Bayesian approach, we furthermore show how to extend this framework to estimate the entire distribution of motility parameters in heterogeneous populations of particles efficiently.

BP 14.7 Wed 12:00 ZEU 160

Derivation and analysis of a phase field crystal model for a mixture of active and passive particles[⋆] — •Michael te Vrugt[1,2], Max Philipp Holl[1], Aron Koch[1], Raphael Wittkowski[1,2,3], and Uwe Thiele[1,3,4] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Center for Soft Nanoscience — [3]Center for Nonlinear Science — [4]Center for Multiscale Theory and Computation

We discuss an active phase field crystal (PFC) model that describes a mixture of active and passive particles [1]. First, a microscopic derivation from dynamical density functional theory is presented that includes a systematic treatment of the relevant orientational degrees of freedom. Of particular interest is the construction of the nonlinear and coupling terms. This allows for interesting insights into the microscopic justification of phenomenological constructions used in PFC models, the approximations required for obtaining them, and possible generalizations. Second, the derived model is investigated using linear stability analysis and nonlinear methods. It is found that the model allows for a rich nonlinear behavior with states ranging from steady periodic and localized states to various time-periodic states. The latter include standing, traveling, and modulated waves corresponding to spatially periodic and localized traveling, wiggling, and alternating peak patterns and their combinations.

[1] MtV et al., Modelling Simul. Mater. Sci. Eng. 30, 084001 (2022)

[⋆]*Funded by the Deutsche Forschungsgemeinschaft (DFG)–WI 4170/3-1*

BP 14.8 Wed 12:15 ZEU 160

Active Brownian Particles in a disordered motility environment — Gianni Jacucci[1], •Davide Breoni[2], Sandrine Heijnen[3], Hartmut Löwen[2], Giorgio Volpe[3], and Sylvain Gigan[1] — [1]Laboratoire Kastler-Brossel, Paris, France — [2]HHU Universität, Düsseldorf, Germany — [3]University College London, London, United Kingdom

The study of active matter, i.e. matter that consumes energy to perform actions, is fundamental to deepen the knowledge of living systems, as for example bacterial colonies or flocks of birds, and their collective behaviors. Complex environments, like the internal structure of a cell or a blood vessel, are of particular relevance in this field, as they provide a better description of the real-life settings typical of living matter.

In this work we study the effects of a disordered motility field on active Brownian particles, both in experiments and simulations. Experimentally, the motility field is generated by applying a speckle light field to thermophoretic Janus particles, in our case silica colloids half-coated with a carbon layer, suspended in a critical mixture of water and 2,6-lutidine. We focus on the differences between the effects of respectively a homogeneous and a disordered motility field on the dynamics of the particles.

BP 14.9 Wed 12:30 ZEU 160

Characterization of spatial heterogeneities as influencing factors on the dynamics of confluent endothelial cell migration — •Anselm Hohlstamm, Andreas Deussen, Stephan Speier, and Peter Dieterich — Institut für Physiologie, TU Dresden

Confluent endothelial cells are in perpetual movement. Their collective dynamics arises from the interplay of self-propelled motility and various distance-related cell interactions. However, an understanding of collective cell dynamics is complicated by large spatial heterogeneities and local cluster formations. It is the aim of this work to quantify and characterize their influence on the dynamics of cell migration. We used human umbilical vein endothelial cells, which were stained with a fluorescent dye and observed for 48 hours via time-lapse microscopy. With automated image segmentation we could track several 10.000 cells. Cell densities and mean squared velocities showed a heterogeneous spatial distribution with an inverse relation to each other. Higher cell densities also affected the strength of the velocity autocorrelation, whereas correlation times remained mostly stable during experiments. However, cell division increased the mean squared velocity without changing temporal correlations. In parallel, the mean squared displacement characterized regions with short superdiffusive phases in an aging, highly non-stationary system. In addition, local dynamics are coupled by long range spatial correlations. In summary, the dynamics of an entire endothelial layer is influenced by interactions of small heterogenous regions. Next, we will use this approach to compare different endothelial cells.

BP 14.10 Wed 12:45 ZEU 160

Exploiting the unknown - Smart nutrient collection surpassing the run and tumble strategy — •Mahdi Nasiri, Edwin Loran, and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

Throughout evolution, microorganisms have developed efficient strategies for locating nutrients and avoiding toxins in complex environments. Understanding their adaptive policies can provide new key insights for the development of smart artificial active particles. In this talk, we will present a novel method that uses deep reinforcement learning (DRL) to develop smart nutrient collection strategies for chemotactic active particles. Our method is complementary to our previous work which used DRL to explore optimal navigation [1] and is able to devise efficient survival strategies inside unknown and complex environments while only having access to local sensory data. We were also able to extract an interpretable model from the learned strategies which resemble striking similarities with the classical run and tumble motion.

[1] M. Nasiri, B. Liebchen, New J. Phys. 24, 073042 (2022).

BP 15: Tissue Mechanics II

Time: Wednesday 10:30–12:15 Location: BAR Schö

BP 15.1 Wed 10:30 BAR Schö

Hydrostatic pressure and lateral actomyosin tension control stretch and tension of the basement membrane in epithelia — •Karla Yanin Guerra Santillan[1,3], Elisabeth Fischer-Friedrich[1,2], and Christian Karla Yanín[1,3] — [1]Cluster of Excellence Physics of Life, Technische Universität Dresden, Dresden, Germany. — [2]Biotechnology Center, TU Dresden, Tatzberg, 01307 Dresden, Germany — [3]School of Science, Technische Universität Dresden, Dresden, Germany

The shaping of epithelial tissues into functional organs often depends on asymmetries in mechanical tension present at the apical and basal sides of cells. Contraction of an actomyosin meshwork underlying the apical side of cells is known to generate apical tension. The basal side of cells is also associated with an actomyosin meshwork, but it is, in addition, connected to a specialized extracellular matrix, the basement membrane. However, how basal tension is generated, and the role of the basement membrane in this process, are often disregarded and not well understood. Here, using atomic force microscopy, we measure mechanical tension in the basal surface of the wing disc epithelium of Drosophila. We find that basal tension depends crucially on the basement membrane with additional contributions of the actomyosin cytoskeleton. Further, performing localized optogenetic activation of actomyosin contractility and osmotic shocks, we deduce that elastic basement membrane stretch is generated by intracellular hydrostatic pressure and lateral actomyosin contractility.

BP 15.2 Wed 10:45 BAR Schö

Noisy growth and buckling in soft tissues — •Rahul G. Ramachandran[1], Ricard Alert[1,2], and Pierre A. Haas[1,2,3] — [1]Max Planck Institute for the Physics of Complex System, 01187 Dresden, Germany — [2]Center for Systems Biology Dresden, 01307 Dresden, Germany — [3]Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany

The generation of curved tissue shapes such as the villi of the gut or the gyrations of the brain has been associated with buckling instabilities that release elastic stresses accumulated by constrained growth. However, most mechanical theories for these morphogenetic processes assume homogeneous growth and mechanical properties, while these parameters often exhibit strong fluctuations in biological systems. Here, we therefore study a minimal mechanical model of these fluctuations: We analyze the buckling of a growing, neo-Hookean rod through nonlinear finite-element simulations. Fluctuations are introduced as spatial inhomogeneities of the growth tensor and the material parameters. Our results show that stronger growth fluctuations promote buckling by decreasing the buckling threshold. We interpret these results using strain energy distribution from homogenous, patterned and random growth simulations and validate them using analytical calculations.

BP 15.3 Wed 11:00 BAR Schö

Viscoelastic measurements in glioblastoma-infiltrated cerebral organoids — •Michael Frischmann[1], Elijah Shelton[1], Sofia Kalpazidou[2], Jovica Ninkovic[2,3], and Friedhelm Serwane[1,3] — [1]Faculty of Physics and Center for NanoScience, LMU Munich, Germany — [2]Biomedical Center, LMU Munich, Germany — [3]Munich Cluster for Systems Neurology, Munich, Germany

The glioblastoma is a malignant neuroepithelial brain tumor with median survival rates of a few months without treatment. One reason is the rapid infiltrative growth with active destruction of brain tissue and the resulting necrotic debris. Glioblastomas are well described from a molecular biology perspective. However, little is known about their mechanical properties which directly affect the tumor's ability to spread into adjacent tissues. I will present measurements of mechancial properties of glioblastoma and its surrounding tissue. To study tumor biophysics in an accessible in vitro system, we use cerebral organoids grown from induced pluripotent stem cells (iPSCs) with implantet glioblastoma cells. To determine the mechancial properties of the tumor and its microenvironment, we use magnetic microdroplets that we inject into the tissue via microneedles. Actuated by a homogeneous magnetic field, the droplet deforms and its deformation is recorded via a confocal microscope. The dynamic deformation is used to infer the viscoelastic properties of physiological and pathological tissue, as well as boundary regions. The recorded data allows us to establish a viscoelastic model of glioblastoma and to develop a mechanical understanding how brain tumors infiltrate their environment.

15 min. break

BP 15.4 Wed 11:30 BAR Schö

Density-dependent active flow transition of biological tissues — •Mathieu Dedenon[1,2], Carles Blanch-Mercader[3], and Karsten Kruse[1,2] — [1]Department of Biochemistry, University of Geneva, 1211 Geneva, Switzerland — [2]Department of Theoretical Physics, University of Geneva, 1211 Geneva, Switzerland — [3]Laboratoire Physico-Chimie Curie, Institut Curie, Université PSL, Sorbonne Université, CNRS UMR168, Paris, France

Biological tissues of elongated cells can spontaneously flow thanks to active stresses, as predicted by 2D generalized hydrodynamics. This effect has been recently confirmed experimentally with confined C2C12 myoblasts.

Under circular confinement, those cells are observed to undergo tissue rotation at confluence. Cells have maximal orientational order at the disc periphery, forming a spiral +1 topological defect. However at

a later stage, cell density increases and the tissue ceases rotational motion. This transition is accompanied by a reorientation of cells along the radial direction, transforming the +1 defect into a static aster.

To understand density-dependent spiral-aster transitions, we generalize the previously used 2D polar active fluid description to incorporate a generic passive coupling between cell density and polarity fields. Using symmetry arguments, several energy terms are allowed and we explore systematically how such couplings affect the spontaneous flow transition, under which conditions they promote a spiral-aster transition. This work shows that collective motion is not only driven by tissue active stress but is also sensitive to cell density.

BP 15.5 Wed 11:45 BAR Schö

Capturing the mechanosensitivity of cell proliferation in models of epithelium — •Maxime Hubert[1], Kevin Höllring[1], Lovro Nuić[2], Luka Rogić[2], Sara Kaliman[1], Simone Gehrer[1], Florian Rehfeldt[3,4], and Ana-Sunčana Smith[1,2] — [1]FAU Erlangen-Nürnberg, Erlangen, Germany — [2]Ruđer Bošković Institute, Zagreb, Croatia — [3]University of Göttingen, Göttingen, Germany — [4]University of Bayreuth, Bayreuth, Germany

The proliferation of epithelial cells, the process of cell growth and cell division, is affected by the mechanical properties of the surrounding environment. While an extensive literature covers single cell mechanoresponse, information about tissue-wide mechanoresponse are scarce. It is only known that high cell density restricts proliferation and eventually leads to homeostasis. In this presentation, we aim at completing the existing literature by addressing the role of both cell density and extracellular stiffness in the proliferation of cells in epithalial monolayer. Using MDCK-II epithelial tissues stained with EdU we are able to measure the fraction of dividing cells at a given cell density and quantify mechanoresponse. We build a cell-level theory of proliferation based on a two-population description which is compared successfully to the experiments and implemented into simulations. Using experiments and simulations, we also address the role of proliferation in the large scale growth of tissues. A tissue-scale theory of epithelial growth based on the cell-level findings is finally presented. This work provides a first step towards a complete description of proliferation at the tissue scale and its influence on its compartmentalization.

BP 15.6 Wed 12:00 BAR Schö

Quantitative 3D live-imaging of self-organisation in embryonic organoids — •Valentin Dunsing, Sham Tlili, Claire Chardès, Léo Guignard, and Pierre-François Lenne — IBDM & CENTURI, Aix-Marseille University/ CNRS, Marseille, France

The emergence of asymmetries within a mass of equivalent cells is the starting event in the development of embryos, resulting in the formation of the main body axes. Despite its fundamental role, the mechanisms that induce symmetry breaking remain largely unknown because they are difficult to probe in vivo, particularly in mammalian embryos. A promising in vitro model to study such mechanisms are embryonic organoids, which undergo gastrulation-like movements similar to those observed in embryos. We aim to use live imaging to disentangle the interplay between signaling, cell differentiation and mechanics underlying self-organized symmetry breaking. Currently available imaging platforms are limited to low-throughput 3D or high-throughput 2D imaging. To overcome this limitation, we establish multi-view single-objective lightsheet microscopy, allowing us to image tens of organoids over hours to days with cellular resolution and sufficient temporal sampling to track cells in 3D. We present ongoing efforts using deep learning based segmentation and quantitative image analysis to correlate cellular dynamics and rearrangements with the expression of key differentiation markers during polarization of aggregates. We thereby analyze how spatially localized expression domains and collective cell movements establish symmetry breaking. Finally, we analyze the variability of spatiotemporal patterns across multiple specimen.

BP 16: Systems Biophysics

Time: Wednesday 11:15–13:00 Location: BAR 0106

Invited Talk BP 16.1 Wed 11:15 BAR 0106

Systems biophysics of bacterial response to cell wall-targeting antibiotics — Rebecca Brouwers[1], Sharareh Tavaddod[1], Leonardo Mancini[2], Jacob Biboy[3], Elizabeth Tatham[1], Pietro Cicuta[2], Waldemar Vollmer[3], and •Rosalind Allen[1,4] — [1]School of Physics & Astronomy, University of Edinburgh, Edinburgh, UK — [2]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [3]Centre for Bacterial Cell Biology, University of Newcastle, Newcastle, UK — [4]Theoretical Microbial Ecology, Faculty of Biological Sciences, University of Jena, Germany

Antibiotics are central in modern medicine, yet bacterial infections are increasingly becoming resistant to antibiotics. To use antibiotics more effectively, we need to understand better how they work. We have used a combination of microbiological and biophysical experiments, and theoretical modelling, to probe how the antibiotic mecillinam, which targets bacterial cell wall synthesis, kills the bacterium Escherichia coli. Comparing killing dynamics under conditions of rich and poor nutrients we conclude that the balance between the rates of creation of cell surface area and volume plays a crucial role in the fate of cells when exposed to this antibiotic.

BP 16.2 Wed 11:45 BAR 0106

Cell size distribution: an analytical comparison between lineage and population experiments — •Arthur Genthon — ESPCI, Université PSL, Paris, France (until december 2022) — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany (from january 2023)

In the past decade, new microfluidic devices, like the mother machine, have been designed to monitor single lineages of cells for many generations with great precision. In classical bulk cultures where full populations are grown, cells with high reproductive success lead to larger populations of offsprings, while no such selection effect is present in single-lineage experiments. Quantifying the statistical bias between these two families of experiments is at the basis of a universal notion of natural selection, which can be defined for any branching tree, not just in cell biology. In this work, we thus compute analytical lineage-population biases for the cell size distribution, in the context of size-controlled cells. The role of stochasticity, both in single-cell growth and in volume partitioning at division, is explored, and we show how it can cancel the lineage-population bias. In addition, in simple cases we show how we can learn the laws of cell growth and division from mother machine steady state size distributions. The parameters of the model, such as the single-cell growth rate, the strength of the size control or the asymmetry of division are obtained by fitting analytical distributions to Escherichia coli data.

BP 16.3 Wed 12:00 BAR 0106

Tuning pattern formation of *E. coli* Min proteins *in vivo* — Ziyuan Ren[1], •Henrik Weyer[2], Laeschkir Würthner[2], Erwin Frey[2], and Suckjoon Jun[1] — [1]Department of Physics & Section of Molecular Biology, Division of Biological Sciences, University of California San Diego, 9500 Gilman Dr. La Jolla, CA 92093, USA — [2]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 München, Germany

The Min protein system of *Escherichia coli* bacteria is crucial for their proliferation. The Min proteins ensure symmetric cell division by positioning the cell-division machinery at midcell. This spatial templating is achieved by the self-organized pole-to-pole oscillation of the Min proteins, suppressing FtsZ ring formation at the cell poles. We experimentally study the robustness of Min pattern formation under changes in the total protein content of MinD and MinE by genetically modifying their expression in live *E. coli* bacteria. This uncovers a remarkable robustness of Min patterns *in vivo* comparable with previous findings *in vitro*. Moreover, this study reveals that the protein concentrations determine the pattern type, and both standing-wave and traveling-wave patterns form in filamentous cells. We show that the same reaction–diffusion model based on the conformational switch of MinE introduced earlier for the *in vitro* system explains both the robustness and the pattern characteristics *in vivo*. Thus, common principles underlie Min pattern formation *in vivo* and *in vitro*.

BP 16.4 Wed 12:15 BAR 0106

Stochastic dynamics of cell shape during cellular state transitions — •Wolfram Pönisch[1], Iskra Yanakieva[1], Aki Stubb[2], Guillaume Salbreux[3], and Ewa Paluch[1] — [1]Dept. of Physiology, Development and Neuroscience, University of Cambridge, Cambridge, UK — [2]Stem Cells and Metabolism Research Program, University of Helsinki, Helsinki, Finland — [3]Dept. of Genetics and Evolution, University of Geneva, Geneva, Switzerland

The development of an organism is characterized by a series of cellular state transitions where cells become increasingly specialized. Such state transitions are often accompanied by morphological changes and there are strong indications of coupling between a cell's shape and state. Here, we present a pipeline to quantify and analyse cell shapes as cells undergo the epithelial-to-mesenchymal transition (EMT). We apply our analysis pipeline to study how shape and fate are coupled during the EMT of MDCK cells. We confirm that cell morphology is closely associated with the state: While epithelial cells display spherical shapes, mesenchymal cells undergo spreading. After defining the distinct cellular shapes corresponding to cell states, we study how exactly the morphological features of a cell evolve during EMT. To this aim, we investigate trajectories of the morphological features of individual cells in a low-dimensional morphospace and describe the evolution of cellular shape as a Langevin process, allowing us to entangle the role of deterministic and stochastic morphogenetic forces. By integrating morphometric analysis into studies of cell state transitions, we aim to better understand the crosstalk between cell state and shape.

BP 16.5 Wed 12:30 BAR 0106

Sensitivity of Boolean attractors to small network changes and implications for the inference of microbial interaction networks — •Jyoti Jyoti and Marc-Thorsten Hütt — Jacobs university, Bremen, Germany

Sensitivity of dynamics on graphs under small topological changes has been studied for diverse types of dynamics and in relation with a wide range of applications. Here we extend this direction of research by studying (and deciphering) the change of attractors in Boolean threshold dynamics under single and multiple edge switches. By evaluating differences in attractor sets, we can, with high accuracy, predict the structural change in the network. This is of high relevance for network inference, e.g., inferring microbial interactions from abundance patterns: Current approaches, where interaction networks are inferred from attractors [1], often fail to provide networks, which in turn can reproduce the initial attractor set. Evaluating the differences in attractor sets (initial set vs. the one produced by the inferred network) and estimating topological differences from them can pave the way towards better inference algorithms. We briefly discuss the implications of our findings for microbiome analyses.

[1] Claussen, J. C., Skiecevičienė, J., Wang, J., Rausch, P., Karlsen, T. H., Lieb, W., Baines, J. F., Franke, A., and Hütt, M.-Th. (2017). Boolean analysis reveals systematic interactions among low-abundance species in the human gut microbiome. *PLoS Computational Biology*, 13(6):e1005361.

BP 16.6 Wed 12:45 BAR 0106

Information storage allows for optimal adaptation in chemical signalling networks out-of-equilibrium — •Daniel Maria Busiello[1] and Giorgio Nicoletti[2] — [1]Max Planck Institute for the Physics of Complex Systems, Germany — [2]University of Padua, Italy

Living systems process information and exhibit dynamical adaptation. We propose a chemical model for sensing that encompasses only necessary ingredients: energy consumption, information storage, and negative feedback. Indeed, equilibrium constraints limit the efficiency of information processing, and storage is an unavoidable energy-consuming step to exploit information. Our model architecture is informed by experimental observations that found negative feedback to be ubiquitous. We show that the presence of information storage and negative feedback leads to finite-time memory, essential for dynamical adaptation. Surprisingly, adaptation is associated with both an increase in the mutual information between external and internal variables and a reduction of dissipation in the internal chemical processes. This twofold advantage comes at an energetic cost. By simultaneously optimising energy consumption and information processing features, we find that far-from-equilibrium sensing dominates in the low-noise regime. Finally, we employ our model to shed light on the adaptation of neurons in zebrafish larvae subjected to periodic visual stimuli. We find striking similarities between predicted and observed behaviours, quantifying dissipation and information-processing performance. Our theory provides a stepping stone towards the idea of highlighting crucial ingredients for information processing starting from a chemical description.

BP 17: Protein Structure and Dynamics

Time: Wednesday 15:00–17:30 Location: BAR 0106

BP 17.1 Wed 15:00 BAR 0106

Computational Approaches to Liquid-Liquid Phase Separation of Partially Disordered RS-Proteins — •Yannick Witzky[1], Stephan Hobe[2], Andreas Wachter[2], Arash Nikoubashman[1], and Friederike Schmid[1] — [1]Institute of Physics, Johannes Gutenberg University — [2]Institute for Molecular Physiology, Johannes Gutenberg University

RS-proteins are a class of proteins that contribute to light-activated gene regulation (via an alternative splicing mechanism) in plant morphogenesis. It has been hypothesized that liquid-liquid phase separation (LLPS) plays an important role for the regulation mechanism. Studying these proteins is challenging because they contain both intrinsically disordered regions (IDRs) - which presumably control the LLPS - as well as folded domains that contain the functionally important RNA binding sites. Here we use and compare different coarse-grained models to study the condensation and phase behavior of RS proteins: Commonly used IDP models [1,2] as well as the structure predictive UNRES model [3]. We specifically focus on the on the single-chain conformations, phase behavior and the accessibility of RNA binding site.

[1] Tesei et al. (2022) Open Research Europe, 2(94), 94.
[2] Rizuan et al. (2022) J Chem Inf Model 62(18), 4474-4485.
[3] Sieradzan et al.(2019) J. Phys. Chem. B, 123, 27, 5721-572

BP 17.2 Wed 15:15 BAR 0106

Key Role of the Solvent in Driving Liquid-Liquid Phase Separation — •Ellen Adams[1,2], Jonas Ahlers[3], Verian Bader[3], Simone Pezzotti[3], Konstanze Winkhofer[3], Jörg Tatzelt[3], and Martina Havenith[3] — [1]Technische Universität Dresden — [2]Hemholtz Zentrum Dresden Rossendorf — [3]Ruhr Universität Bochum

In recent years the importance of the aqueous solvent in influencing protein structure, function, and dynamics has been recognized. Coupling of water molecules to the protein surface creates an interfacial region in which water molecules within this region have distinctly different properties than bulk water. Yet, the structure and dynamics within this interfacial region are still not easy to access experimentally. Terahertz (THz) spectroscopy has been shown to be a powerful tool to investigate solvent dynamics in bulk solutions and is directly sensitive to changes in the low frequency collective intermolecular hydrogen-bonding vibrations of water. Here the role of solvation dynamics in the liquid-liquid phase separation (LLPS) of the intrinsically disordered protein fused in sarcoma (FUS) is probed. Characterization of the hydrogen bonding network reveals that water solvating hydrophobic groups is stripped away in the membrane-less FUS biomolecular condensates. Additionally, water left inside of the biomolecular condensates is highly constrained, indicative of a population of bound hydration water. These results uncover the vital role of hydration water in LLPS: the entropically favorable release of unfavorable hydration water serves as a driving force for LLPS.

BP 17.3 Wed 15:30 BAR 0106

Local structure and dynamics of water molecules in FUS protein molecular condensates. — Daniel Chavez Rojas[1], •Joseph Rudzinski[1,2], and Martin Girard[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany

There is evidence that molecular condensates of the FUS protein play a role in the development of some neurodegenerative diseases like ALS. For this reason, understanding the molecular mechanism by which

these condensates form at an atomistic level is of therapeutic interest. However, the molecular structure and water-protein interactions of these condensates is poorly understood. In this work, we utilize a multi-scale approach to generate FUS condensates at a sufficient scale with a coarse-grained model, followed by investigation of the atomic scale with shorter, fully-atomistic molecular dynamics simulations. As a result, we are able to efficiently characterize water-protein hydrogen bonding interactions, contacts, and water ordering around the individual amino acids of FUS proteins in the condensate versus in solution. The characterization of water-protein and protein-protein structure provides insights about the driving forces that promote the formation of these molecular condensates.

BP 17.4 Wed 15:45 BAR 0106

Structural dynamics of the intrinsically disordered SNARE proteins at the membrane interface: Recent insights by NMR spectroscopy — Tobias Stief[1,2], Mirko Kraus[1,2], Katharina Vormann[1,2], Reinhard Jahn[3], Angel Perez-Lara[4], and •Nils-Alexander Lakomek[1,2] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Heinrich-Heine-Universität, Düsseldorf, Germany — [3]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [4]University of Granada, Granada, Spain

SNARE proteins play a crucial role during neurotransmitter release by eliciting the fusion of the synaptic vesicle membrane with the presynaptic plasma membrane. In their pre-fusion state, the SNARE proteins are intrinsically disordered. They do not exhibit a well-defined structure and show high internal flexibility, being membrane-anchored. However, the mode of interaction between the SNARE proteins and the lipid membrane needs to be better understood.

We use the SNARE proteins as a model system for developing novel NMR methods to characterize the inner and conformational dynamics of intrinsically disordered proteins interacting with lipid membranes or being membrane-anchored. Therefore, we address a large range of timescales, from pico- to milliseconds, employing both solution NMR and solid-state NMR methods. The aim is to better describe the conformational space of intrinsically disordered proteins at the lipid membrane interface. At the conference, we will present recent (unpublished) insights into the structural dynamics of the SNARE protein synaptobrevin-2 at the lipid membrane interface.

BP 17.5 Wed 16:00 BAR 0106

Single-chain and condensed-state behavior of intrinsically disordered nuclear proteins in bulk and confinement — •Janka Bauer[1], Lukas Stelzl[1,2,3], Dorothee Dormann[2,3], and Arash Nikoubashman[1] — [1]Institute of Physics, JGU Mainz, Germany — [2]Biocenter, Institute of Molecular Physiology, JGU Mainz, Germany — [3]Institute of Molecular Biology, Mainz, Germany

The liquid-liquid phase separation of intrinsically disordered proteins plays an integral part for the formation of membraneless organelles in cells, which in turn have key functional and regulatory roles. To better understand the complex relation between the sequence and self-assembly of these heteropolymers, we perform molecular simulations of the low-complexity domains of heterogeneous nuclear ribonucleoprotein A1 (hnRNPA1) and Fused in Sarcoma (FUS). For hnRNPA1, we systematically analyze how the conformation and phase behavior are affected by the number of aromatic residues within the examined sequences in both single-chain and condensed state simulations. Our observations strongly support the hypothesis that aromatic residues play a dominant role for condensation, which is further corroborated by a detailed analysis of the intermolecular contacts. To mimic more closely conditions prevalent in cellular environments, we perform simulations of hnRNPA1 and FUS in spherical confinement, where we systematically vary the fraction of the crowding agent polyethylene glycol.

15 min. break

BP 17.6 Wed 16:30 BAR 0106

Efficiency and selectivity in the self-assembly of SAS-6 rings on a surface — •Santiago Gomez Melo[1], Dennis Wörthmüller[1], Pierre Gönczy[2], Niccolo Banterle[3], and Ulrich Schwarz[1] — [1]Heidelberg University, Heidelberg, Germany — [2]EPFL, Lausanne, Switzerland — [3]EMBL, Heidelberg, Germany

Centrioles are large cylindrical structures that organize various microtubule-based processes in cells, including the formation of cilia and spindles. Their characteristic nine-fold symmetry results from rings that are formed by dimers of the protein SAS-6. Recently it was observed that the self-assembly of SAS-6 rings is strongly facilitated on a surface. Moreover, a fraction of non-canonical symmetries (i.e., different from nine) was observed. To better understand the factors that determine the efficiency and selectivity of this process, we have performed Brownian Dynamics computer simulations with patchy particles, in which we varied interaction energies and angular binding range. For weak interaction energies and large angular range, we find that the assembly kinetics can be described well by the coagulation-fragmentation equations in the reaction-limited approximation. In contrast, large interaction energies and small angular range lead to kinetic trapping and diffusion-limited assembly. Comparison with experimental data suggests that the SAS-6 system combines a weak binding energy with a small angular range in order to avoid kinetic trapping and favor the desired nine-fold symmetry.

BP 17.7 Wed 16:45 BAR 0106

Alphafold predicts the most complex protein knot and composite protein knots — Maarten Brems[1], Robert Runkel[1], Todd Yeates[2], and •Peter Virnau[1] — [1]Institut für Physik, Staudingerweg 9, JGU Mainz — [2]UCLA-DOE Institute for Genomics and Proteomics, University of California Los Angeles (USA)

The computer artificial intelligence system AlphaFold has recently predicted previously unknown three-dimensional structures of thousands of proteins. Focusing on the subset with high-confidence scores, we algorithmically analyze these predictions for cases where the protein backbone exhibits rare topological complexity, i.e. knotting. Amongst others, we discovered a 7_1-knot, the most topologically complex knot ever found in a protein, as well as several 6-crossing composite knots comprised of two methyltransferase or carbonic anhydrase domains, each containing a simple trefoil knot [1]. These deeply embedded composite knots occur evidently by gene duplication and interconnection of knotted dimers. Finally, we report two new five-crossing knots including the first 5_1-knot. Our list of analyzed structures forms the basis for future experimental studies to confirm these novel knotted topologies and to explore their complex folding mechanisms.

[1] M. Brems et al, Protein Science 31(8), e4380 (2022).

BP 17.8 Wed 17:00 BAR 0106

Multi-state Unfolding Processes: Discrimination of protein domains by urea-induced thermal shift — •Ji Young Yang[1,2], Oliver Burkert[2], Boris Mizaikoff[1], and Jens Smiatek[3,4] — [1]Institute for Analytical and Bioanalytical Chemistry, University of Ulm, Ulm, Germany — [2]Boehringer Ingelheim Pharma GmbH & Co. KG, Analytical Development Biologicals, Biberach(Riss), Germany — [3]Boehringer Ingelheim Pharma GmbH & Co. KG, Development NCE, Biberach (Riss), Germany — [4]Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

Co-solute induced molecular denaturation and aggregation mechanisms related to stability changes for multi-domain proteins like mAbs are often hard to monitor experimentally. In addition, a thorough theoretical explanation is often missing. We performed intrinsic fluorescence (IF) measurements of monoclonal antibody (mAb) samples for different aqueous urea concentrations under thermal denaturation. Our results show that the denaturating effect of urea on individual mAb domains can be explained by linear mapping of the thermal shifting curve to the actual urea concentration. Notably, the achieved thermal shifting curves can be assigned to certain protein domains, which enables discrimination of overlapping denaturation processes. Our approach highlights the benefits of direct monitoring of co-solute effects on the conformational stability of mAb domains and its colloidal stability. We will discuss the experimental approach and present the corresponding outcomes in terms of the underlying molecular mechanisms.

BP 17.9 Wed 17:15 BAR 0106

X-ray damage to Gene-V Protein: NAP-XPS analysis of Chemical changes to Proteins in Water — •Dorothea C Hallier[1,2,3], Jörg Radnik[2], Paul M Dietrich[4], Harald Seitz[1,3], and Marc Benjamin Hahn[2] — [1]Fraunhofer Insitute for Cell Therapy and Immunology, Branch Bioanalytics and Bioprocesses, Potsdam, Germany — [2]Federal Insitute for Materials Research and Testing BAM Berlin, Berlin, Germany — [3]Univerity of Potsdam, Institute for Biochemistry and Biology, Potsdam Germany — [4]SPECS Surface Nano Analysis GmbH, Berlin, Germany

X-ray photoelectron spectroscopy (XPS) was used to analyze the chem-

ical damage of ionizing radiation to a single-stranded DNA-binding protein: Gene-V Protein (G5P/GVP) and its most abundant amino acids (Alanine, Arginine, Cysteine, Glycine, Lysine, Methionine, Tyrosine). This protein plays a crucial role in maintaining the DNA metabolism, especially DNA replication, recombination and repair. Vacuum measurements were combined with near-ambient pressure (NAP) XPS measurements under water and nitrogen atmosphere to detect both direct and indirect radiation damage and corresponding damage pathways. The exposure of proteins and aminoacids to x-rays leads to degradation i.e. via dehydrogenation, decarboxylation, dehydration and deamination. A strong increase of protein damage was observed in water as compared to vacuum.

BP 18: Biologically Inspired Statistical Physics (joint session DY/BP)

Time: Wednesday 15:00–16:30 Location: ZEU 250

BP 18.1 Wed 15:00 ZEU 250

Comparison of fitting strategies to extract the diffusion coefficient in microrheological experiments — •Sten Leipnitz, Christian Wagner, and Thomas John — Experimental Physics, Saarland University, Saarbrücken

Tracking of small particles undergoing a Brownian motion in liquids is a widespread method in passive microrheology to extract the diffusion coefficient D, the viscosity of the sample respectively. The mean-squared displacement (MSD) is determined from particle positions as a function of the timelag $MSD(\tau) = \sigma_0^2 + 2nD\tau + v_{\mathrm{drift}}^2\tau^2$, where v_{drift} is a possible drift velocity and σ_0 is an offset due to position detection noise in experiments. We present: the extracted parameters depend strongly on the used number of fitting points in the MSD-relation. Surprisingly, considering only the beginning of the MSD-relation in the fitting procedure leads to the best expectation value of the diffusion coefficient. This is shown by numerical simulations of the Brownian motion as well as from experimental data.

BP 18.2 Wed 15:15 ZEU 250

Non-monotonic behavior of timescales of passage in heterogeneous media: Dependence on the nature of barriers — Moumita Dasgupta[1], •Sougata Guha[2], Leon Armbruster[1], Dibyendu Das[2], and Mithun K. Mitra[2] — [1]Department of Physics, Augsburg University, USA — [2]Department of Physics, IIT Bombay, India

Usually time of passage across a region may be expected to increase with the number of barriers along the path. Can this intuition fail depending on the special nature of the barrier? We study experimentally the transport of a robotic bug which navigates through a spatially patterned array of obstacles. Depending on the nature of the obstacles we call them either entropic or energetic barriers. For energetic barriers we find that the timescales of first passage vary non-monotonically with the number of barriers, while for entropic barriers first passage times increase monotonically. We perform an exact analytic calculation to derive closed form solutions for the mean first passage time for different theoretical models of diffusion. Our analytic results capture this counter-intuitive non-monotonic behaviour for energetic barriers. We also show non-monotonic effective diffusivity in the case of energetic barriers. Finally, using numerical simulations, we show this non-monotonic behaviour for energetic barriers continues to hold true for super-diffusive transport. These results may be relevant for timescales of intra-cellular biological processes.

BP 18.3 Wed 15:30 ZEU 250

Phase behavior and finite-size effects in biology — •Felix Hermann, Burkhard Duenweg, and Martin Girard — Max-Planck Institut fuer Polymerforschung (MPI-P), Mainz, Germany

Phase behavior observed in biology remains puzzling. For instance, the plasma membrane of cells exhibits signs of criticality, as it is controlled to remain near a demixing point. This membrane contains thousand of components, and it is largely unclear how its composition is controlled. Beyond this, one can ask whether cells should obey the traditional thermodynamic picture, given their small size, large number of components and the presence of non-equilibrium processes.

Here, we study toy systems, lattice models containing many (>30) components. We show that these systems exhibit strong finite-size effects. These manifest as behavior that appears similar to traditional critical behavior, but vanish logarithmically with system size. We examine scaling laws, and whether traditional paradigms from macroscopic thermodynamics can be broken in such systems.

BP 18.4 Wed 15:45 ZEU 250

Hierarchical interactions in complex ecosystems — •Lyle Poley[1], Joseph W. Baron[3], and Tobias Galla[1,2] — [1]Theoretical Physics, Department of Physics and Astronomy, School of Natural Sciences, The University of Manchester, Manchester M13 9PL, UK — [2]Instituto de Física Interdisciplinar y Sistemas Complejos IFISC (CSIC-UIB), 07122 Palma de Mallorca, Spain — [3]Laboratoire de Physique Statistique, École Normale Supérieure (ENS), Paris Sciences et Lettres (PSL) Research University, Sorbonne Université, 75005 Paris, France

In the analysis of complex ecosystems it is common to use random interaction coefficients, often assumed to be such that all species are statistically equivalent. We relax this assumption by imposing hierarchical inter-species interactions, which we incorporate into a generalised Lotka-Volterra dynamical system. These interactions impose a hierarchy in the community. Species benefit more, on average, from interactions with species below them in the hierarchy than from interactions with those above.

Using analytical tools from the theory of disordered systems, most notably path-integrals and dynamic mean-field theory, we demonstrate that a stronger hierarchy stabilises the community by reducing the number of species in the surviving community. We will also show that the probability of survival for a given species is dependent on its position in the hierarchy.

Reference: Poley L, Baron J W and Galla T Generalised Lotka-Volterra model with hierarchical interactions 2022 arXiv:2208.01569

BP 18.5 Wed 16:00 ZEU 250

Quantifying information content in continuous attractor networks — •Tobias Kühn[1,2] and Rémi Monasson[1] — [1]Laboratoire de Physique de l'Ecole Normale Supérieure, ENS, Université PSL, CNRS, Sorbonne Université, Université Paris Cité, F-75005 Paris — [2]Institut de la Vision, Sorbonne Université, INSERM, CNRS, F-75012 Paris

Attractor networks are a theme with long tradition to model information storage in the brain. Continuous attractor neural networks (CANN), in particular, have been employed to describe the storage of information about space and orientation. However, it stays controversial how useful this paradigm really is to explain actual processes, for example the representation of space in grid and place cells in the entorhinal cortex and the hippocampus, respectively.

A common criticism is that the disorder present in the connections might deteriorate the system's capability to reliably preserve the information of a certain pattern. In order to investigate if this criticism is valid, a measure is needed to objectively quantify the information content of a given neural network. Using the replica-trick, we compute the Fisher information for a network receiving space-dependent input whose connections are composed of a distance-dependent and a disordered component. We observe that the decay of the Fisher information is slow for not too large disorder strength, indicating that CANNs have a regime in which the advantageous effects of connectivity on information storage outweigh the detrimental ones.

BP 18.6 Wed 16:15 ZEU 250

Gift of gab: Probing the limits of dynamic concentration-sensing across a network of communicating cells — •Mohammadreza Bahadorian[1,2], Christoph Zechner[1,2,3], and Carl D. Modes[1,2,3] — [1]Max Planck Institut for Molecular Cell Biology and Genetics (MPI-CBG), 01307 Dresden, Germany — [2]Center for Systems Biology Dresden (CSBD), 01307 Dresden, Germany — [3]Cluster of Excellence Physics of Life, TU Dresden, 01069 Dresden, Germany

Many systems in biology and other sciences employ collaborative, collective communication strategies for improved efficiency and adaptive benefit. One such paradigm of particular interest is the community

estimation of a dynamic signal, when, for example, an epithelial tissue of cells must decide whether to react to a given dynamic external concentration of stress-signaling molecules. At the level of dynamic cellular communication, however, it remains unknown what effect, if any, arises from communication beyond the mean field level. What are the limits and benefits to communication across a network of neighbor interactions? What is the role of Poissonian versus super-Poissonian dynamics in such a setting? How does the particular topology of connections impact the collective estimation and that of the individual participating cells? In this article we construct a robust and general framework of signal estimation over continuous-time Markov chains in order to address and answer these questions.

BP 19: Biopolymers, Biomaterials and Bioinspired Functional Materials (joint session CPP/BP)

Time: Wednesday 16:30–18:00 Location: MER 02

BP 19.1 Wed 16:30 MER 02

Low-Temperature and Water-Based Biotemplating of Nanostructured Foam-Like Titania Films using ß-Lactoglobulin — •Julian E. Heger[1], Wei Chen[1], Shanshan Yin[1], Nian Li[1], Volker Körstgens[1], Calvin J. Brett[2,3], Wiebke Ohm[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]DESY, Hamburg, Germany — [3]Royal Institute of Technology KTH, Stockholm, Sweden — [4]MLZ, TUM, Garching, Germany

Energy-related applications such as solar cells, batteries, and the photocatalytic production of hydrogen are broadly built up on titania nanostructures. A tailored titania morphology is necessary to match the required charge diffusion lengths and the crystallinity beneficial for efficient performance. In the context of large-scale fabrication, the aspect of sustainability becomes essential. Biopolymer templating based on ß-Lactogobulin (ß-lg) and spray deposition promotes low-temperature and water-based synthesis of nanostructured, crystalline, foam-like titania films. During spray deposition, the ß-lg biopolymer matrix sterically directs the titania morphology. Afterwards, the biotemplate is removed by UV-light exposure. To understand the kinetics of film formation during the spray deposition on the nano and crystalline length scale, we simultaneously perform in situ grazing-incidence small-angle and wide-angle X-ray scattering (GISAXS/GIWAXS). Together with scanning electron microscopy (SEM), the results explain the role of ß-lg as a biotemplate.

BP 19.2 Wed 16:45 MER 02

Structural changes in cellulose nanofibril-colloid hybrid films during humidity cycling — •Stephan V. Roth[1,2], Calvin J. Brett[1,2], Alexandros Alexakis[2], Lucas P. Kreuzer[3], Martin Mansson[2], Sarah Rogers[4], Eva Malmström[2], Peter Müller-Buschbaum[3,5], and L. Daniel Söderberg[2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]KTH Royal Institute of Technology, Stockholm, Sweden — [3]TUM School of Natural Sciences, Chair for Functional Materials, Garching — [4]ISIS-STFC, Rutherford Appleton Laboratory, Chilton, Oxon OX11 0QX, UK — [5]MLZ, TUM, Garching, Germany

Biocompatible cellulose nanofibrils (CNFs) are an ideal material for sustainable biomaterial templates. Combined with latex colloids, the resulting hybrid colloid-CNF functional materials are excellent candidates for bio-inspired structural colors. Due to the hydrophilic nature of CNFs, we investigate the stability against humidity cycling in terms of reversible/irreversible structural rearrangements. We applied depth sensitive grazing incidence small-angle neutron scattering to evaluate the humidity-induced rearrangements in hybrid latex colloid:CNF templates in situ during cyclic humidification. After the first humidity cycle, a change in morphology on the scale of several 10 nm was observed, which is attributed to latex particles which diffused in the network and enlarged the pores of the network. The measured kinetics resolve the time- and depth-dependence of the differently sized colloids' penetration into the porous CNF network.

BP 19.3 Wed 17:00 MER 02

Fluorescence correlation spectroscopy for studying the aggregation of nanoplastics in model biofilm substances — •Tobias Guckeisen, Rozalia Orghici, and Silke Rathgeber — Universität Koblenz, Deutschland

Nanoplastics in the environment are a growing problem. Pollutants can adhere to their surfaces and therefore be easily transported into the natural systems. Biofilms are found everywhere in the environment; they are formed by microbial communities that produce a matrix of extracellular polymeric substances. The interaction between nanoplastics and biofilms can lead to aggregation and sedimentation of nanoparticles and determines the transport and fate of nanoplastics. A better understanding of the transport and fate of nanoplastics is important to improve our ability to predict risks associated with these ubiquitous contaminants. In this project, we use fluorescence correlation spectroscopy (FCS) to study the aggregation and interactions of nanoplastics with model biofilm substances. Protein-polysaccharide mixing ratio and pH-dependent aggregation studies show that it is crucial to consider correlative effects between multiple biofilm components to better understand the impact biofilms have on nanoplastic aggregation. Biofilm model systems with only one component, as commonly considered, may lead to an incorrect assessment of the tendency to aggregation.

BP 19.4 Wed 17:15 MER 02

Ensemble inequivalence and negative extensibility in a wormlike chain with fluctuating bending stiffness — •Panayotis Benetatos — Department of Physics, Kyungpook National University, Republic of Korea

Many semiflexible polymers exhibit fluctuations in the local bending stiffness along their contour. This may be due to intrinsic conformational changes (e.g., denaturation bubble formation in double stranded DNA or helix-coil transition in polypeptides) or to the reversible adsorption and desorption of molecules from the polymer's environment. In this presentation, we analyse the tensile elasticity of a strongly stretched wormlike chain which consists of N concatenated segments, where each segment can be in one of two states, A and B, which differ in bending stiffness. We call this model the reversible wormlike chain (rWLC) model. In the Gibbs (fixed-force, isotensional) ensemble, we obtain analytic expressions for the force-expression relation and the mean fraction of B segments. We show that, under certain conditions, there is a tension-induced crossover from a mostly A to a mostly B rWLC. In the Helmholtz (fixed-extension, isometric) ensemble, we obtain analytic expressions up to a summation. We show that, for finite N, there is marked ensemble inequivalence. Remarkably, in the Helmhlotz ensemble, the rWLC can exhibit negative extensibility and multiple peaks.

BP 19.5 Wed 17:30 MER 02

Aging and compressed exponential stress relaxation in mechanoresponsive hydrogels — •Geonho Song[1,2], Wouter Ellenbroek[3], and Kerstin Blank[1,2] — [1]Johannes Kepler University Linz, Linz, Austria — [2]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [3]Eindhoven University of Technology, Eindhoven, The Netherlands

Biological materials, such as the extracellular matrix (ECM), are viscoelastic and exhibit stress relaxation. Stress relaxation in the ECM is linked to cellular behavior and needs to be considered as a design parameter when developing bioinspired materials for cell culture and tissue engineering. Here, we introduce a collagen-inspired hydrogel with tunable crosslink kinetics. We utilize collagen-mimetic peptides with controlled association and dissociation rates to crosslink star-shaped polyethylene glycol. We show that ultraslow crosslink dissociation rates cause a distinctive relaxation behavior that is reminiscent of soft glassy materials, showing out-of-equilibrium properties. In particular, subjecting the networks to a sequence of pre-stress and aging causes uncommon compressed exponential relaxation. This unique phenomenon has previously only been reported for a small number of soft glassy systems where compressed exponential relaxation was related to ultraslow dynamics that prohibited the release of internal stresses. In such systems, slow crosslink dissociation delays network relaxation until an external trigger is applied. In future work, we aim

to investigate the interplay between locally generated stresses, such as cellular traction forces, and network relaxation properties.

BP 19.6 Wed 17:45 MER 02

Nonaffinity controls critical slowing down and rheology near the onset of rigidity — •Abhinav Sharma[1], Jordan Shivers[2], and Fred MacKintosh[2] — [1]Leibniz institute for polymer research, Dresden — [2]Rice University, Houston, Texas

Fluid-immersed networks and dense suspensions often reside near a boundary between soft (or fluid-like) and rigid (or solid-like) mechanical regimes. This boundary can be crossed either by varying the concentration or by deformation. Near the onset or loss of rigidity, dissipation-limiting nonaffine rearrangements dominate the macroscopic viscoelastic response, giving rise to diverging relaxation times and power-law rheology. Here, we derive a simple relationship between nonaffinity and excess viscosity in fluid-immersed amorphous materials. We then demonstrate this relationship and its rheological consequences in simulations of stress relaxation in strained filament networks and dense suspensions.

BP 20: Members' Assembly

Time: Wednesday 18:00–19:00 Location: BAR Schö

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

BP 21: Bioimaging

Time: Thursday 9:30–13:00 Location: BAR Schö

BP 21.1 Thu 9:30 BAR Schö

Imaging DNA-Origami with Low Energy Electron Holography — •Moritz Edte[1], Hannah Ochner[1], Luigi Malavolti[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Our low-energy electron holography (LEEH) approach makes use of a coherent low-energy electron wave (energies in the range of 50 to 150 eV) for imaging biomolecules with high contrast [1]. Hence, the method allows true single-molecule imaging of large three-dimensional molecules and can map conformational variability of flexible molecules [2]. I will show LEEH measurements of individual DNA-Origami molecules on single layer graphene, demonstrating that LEEH is capable of imaging this class of molecules without introducing perceptible structural changes on the time scale of the measurements and on the spatial scale defined by our current resolution limit.

[1] J.-N. Longchamp, et al., PNAS, 2017, 114, 1474-1479. [2] H. Ochner, et al., PNAS, 2021, 118, e2112651118

BP 21.2 Thu 9:45 BAR Schö

Spectral and nanolocal discrimination of crosslinked from single fibrillar actin using mid-IR photoinduced force microscopy (PiF-IR) — Jesvin Joseph[1,2], Dijo Moonnukandathil Joseph[1,2], Lukas Spantzel[2,3], Katharina Reglinski[1,2], Christoph Krafft[1,2], Christian Eggeling[1,2], Rainer Heintzmann[1,2], Michael Börsch[2,3], and •Daniela Täuber[1,2] — [1]Leibniz Institute of Photonic Technology, Jena — [2]Friedrich Schiller University Jena — [3]Jena University Hospital, Jena, Germany

Fibrillar actin is one of the major structural components in cells. Consequently, pathogenic alterations in cell functionality may be revealed by monitoring the re-arrangement of F-actin. However, discriminating protein aggregation in the range below 10 nm is challenging even by high resolution fluorescence microscopy. This gap can be addressed by recently developed mid-IR photo-induced force microscopy (PiF-IR). PiF-IR spectra obtained from fibrillar and monomeric actin match the corresponding FTIR spectra. The high spectral resolution of PiF-IR provides simplified access to IR spectroscopic signatures from secondary protein structure. The intensity of bands at 1655 cm-1 and 1685 cm-1 associated to α-helices and intermolecular β-sheets, respectively, varied within the scan image. Furthermore, PiF-IR hyperspectra obtained form single fibrillar actin appear more homogeneous than those from cross-linked F-actin. These first results are very promising for using PiF-IR to discriminate F-actin structures to study pathogenic alterations in cells and tissue ex vivo.

BP 21.3 Thu 10:00 BAR Schö

Cryo-EM samples of gas-phase purified protein assemblies using native electrospray ion-beam deposition (ES-IBD) — •Tim Esser[1], Lukas Eriksson[2], Paul Fremdling[2], and Stephan Rauschenbach[2] — [1]Thermo Fisher Scientific, 1 Boundary Park, Hemel Hempstead, HP2 7GE, UK — [2]Department of Chemistry, University of Oxford, Oxford OX1 3TF, UK

Combining native mass spectrometry (MS) with cryo electron microscopy (cryo-EM) allows to correlate information on homogeneity, stoichiometry, shape, and interactions of native protein complexes, complementary to high-resolution protein structures. Cryo-EM samples are conventionally made by coating TEM grids with a protein-containing solution, blotting, and plunge freezing in liquid ethane, quenching proteins in their native state, embedded in ultra-thin films of vitreous ice. Reliable sample preparation remains a major challenge, in particular for heterogeneous samples. Here we demonstrate mass-selective cryo-EM sample preparation via native electrospray ion-beam deposition (ES-IBD), as a direct link between native MS and cryo-EM. Protein complexes are brought into the gas phase, mass-selected, and deposited on TEM grids with thin carbon films at defined temperature. By controlling interactions in solution, gas-phase, and on the surface, we probe protein conformations between native solution-phase and native-like gas-phase structures. We show sub-nanometer EM density maps obtained using native ES-IBD and discuss its potential to extend the scope of cryo-EM in structural biology.

BP 21.4 Thu 10:15 BAR Schö

CRISPR activation screen to improve the optical properties of living tissues — •Susan Wagner, Venkat Krishnaswamy, Kaushikaram Subramanian, Heike Petzold, Benjamin Seelbinder, Rico Barsacchi, and Moritz Kreysing — Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Today, optical microscopes deliver unprecedented resolution allowing discoveries down to the molecular level. Nevertheless, optical access of living biological samples by microscopes is usually restricted to the outer most surface owing to tissue-induced light scattering.

Using directed evolution, we successfully improved the optical properties of mammalian cells. We aim to fully understand this optical plasticity of cells, and genetically clear living mammalian tissues by targeting responsible genes. We are conducting a genome-wide CRISPR activation screen to find genes which confer transparency. This contribution seeks to report on progress, challenges, and opportunities of this technology for biophotonics research, and more generally its potential towards a system level understanding of cellular biophysics.

As a next step, we are investigating how improved optical properties of individual cells influence the optical properties of 3D cell clusters, such as spheroids, using interspersed external fluorescent microspheres to quantify unbiased imaging quality.

Understanding the full potential of the optical plasticity of a tissue bears the potential of providing us with a broad toolkit, so that different genetic strategies can be applied depending on the specific nature of the various biological samples.

BP 21.5 Thu 10:30 BAR Schö

Optical characterization of biological material across scales using interferometric microscopy — •Daniel Midtvedt — Department of Physics, University of Gothenburg

The physicochemical properties, such as size, mass, and composition, of biological matter generally impact its function. However, quantitative characterization of these parameters across the many length-, time-

, and mass scales relevant for biology is challenging. Interferometric imaging techniques, such as holographic imaging and interferometric scattering microscopy (iSCAT), provide quantitative measurements of the light scattering properties of biological objects, and are promising techniques for achieving such characterization. However, although iSCAT provides exquisite sensitivity, quantitatively relating the measured signal to physicochemical properties is straightforward only for small (Rayleigh) scatterers. The holographic signal, on the other hand, can be quantified across arbitrary length scale, but due to poor signal-to-noise ratio it is typically restricted to particles larger than the illuminating wavelength. In this talk, I will showcase some of our recent results combining interferometric imaging techniques with deep learning, enabling pushing the limit of mass quantification in holographic imaging toward the Rayleigh limit, thereby bridging a gap in optical characterization of small particles. With our technique, we are able to characterize biological matter across four orders of magnitude in length, four order of magnitude in time, and ten orders of magnitude in mass. I will highlight the key steps that have enabled us to make this development, and discuss its potential impact on life science research.

BP 21.6 Thu 10:45 BAR Schö

Adaptive optics in Confocal microscopy and Fluorescence correlation spectroscopy — •Julius Trautmann, Philipp Kellner, and Christian Eggeling — Institute for Applied Optics and Biophysics, Friedrich-Schiller University Jena, Philosophenweg 7, 07743 Jena

For more than three decades adaptive optics have been widely used in astronomical applications, but only in recent years it has established itself as an important feature for high resolution microscopy. The ability to correct for optical aberrations can be useful for any kind of setup but it proved particularly useful when imaging samples with inhomogeneous refractive index structures such as cells and especially cell tissue.

The most established adaptive optic elements include deformable mirrors (DMs) and spatial light modulators (SLMs) which can dynamically correct for aberrations.

This talk will cover the basic idea of including a deformable mirror (DM) in a confocal microscope within a fluorescence correlation spectroscopy (FCS) setup. A comparison of placing the deformable mirror in the excitation or detection beam path will take place.

15 min. break

Invited Talk BP 21.7 Thu 11:15 BAR Schö

Visualizing the inner life of microbes — •Ulrike Endesfelder — Institute for Microbiology and Biotechnology, Bonn University, Germany

Microbes, as unicellular organisms, are crucial model systems for the study of cellular mechanisms and functions. With the advent of modern fluorescence microscopy techniques, we can now visualize the inner workings of microbes at the molecular level, e.g. the dynamics of single molecules and the molecular architecture of sub-cellular structures. By quantifying the molecular characteristics of microbes in vivo, we thus can create detailed, spatially and temporally resolved maps of their molecular makeup, allowing us to understand the dynamic heterogeneity and sub-populations at the sub-cellular level. In this talk, I will discuss the potential of single-molecule biophysical approaches for microbiology, using examples from our own research and outlining our future visions.

BP 21.8 Thu 11:45 BAR Schö

A Minimal Model of CD95 Signal Initiation Revealed by Advanced Molecular-Sensitive Imaging — •Nina Bartels[1], Nicolaas TM van der Voort[2], Claus AM Seidel[2], and Cornelia Monzel[1] — [1]Experimental Medical Physics, Heinrich-Heine University, Düsseldorf, Germany — [2]Molecular Physical Chemistry, Heinrich-Heine University, Düsseldorf, Germany

The spatio-temporal organization and dynamic interactions of receptors in the plasma membrane are fundamental for our mechanistic understanding of cell signal initiation. A paradigm of a cell signal initiation process is the ligand-induced oligomerization of TNF (tumor necrosis factor) receptor CD95 in the signaling pathway for apoptosis. Here, we scrutinize proposed CD95 oligomerization models in the cell plasma membrane by applying a molecular sensitive imaging toolkit with up to nanometric resolution including time-resolved FRET spectroscopy, confocal Photobleaching Step Analysis, STED microscopy, and FCS. Covering a wide range of parameters, CD95 interactions are probed over the whole dynamic range from μs to hours, molecular to cellular scales, and with particular focus on quantifying molecular concentrations. Our multiscale study reveals a minimal oligomerization model to trigger apoptosis efficiently, where only ∼8-17% CD95 monomers assemble into dimers/trimers after ligand binding. Further, we highlight the importance of combining complementary techniques for a full understanding of transient and potentially localized processes such as a cell signal initiation.

see also https://doi.org/10.1101/2022.11.29.518370

BP 21.9 Thu 12:00 BAR Schö

Investigating human lung tissue by propagation-based phase-contrast X-ray tomography — •Jakob Reichmann[1], Stijn Verleden[2], Mark Kühnel[3], Jan-Christopher Kamp[3], Lavinia Neubert[3], Jan-Hendrik Müller[1], Thanh Quynh Bui[1], Danny Jonigk[3], and Tim Salditt[1] — [1]Institute for X-ray Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Anatomy and Research Centre, University of Antwerp, Universiteitsplein 1, 2610 Wilrijk, Belgium — [3]Institute of Pathology, Hannover Medical School, Carl-Neuberg-Straße 1, 30625 Hannover

The lung is a perfect example of how the function of an organ is enabled by its three-dimensional structure, here formed by intricate and intertwined networks of ventilation and vasculature. In this work we study the structure of lung tissues over multiple scales down to the sub-cellular level by phase-contrast computed tomography (PCCT). We show how human lung tissues with their largely air-filled compartments and small vessels can be imaged non-destructively with a scalable, isotropic resolution and quantitative density. Three-dimensional reconstructions with varied voxel sizes down to 130nm are obtained by advanced phase retrieval and tomographic reconstruction, shedding light on the three-dimensional cytoarchitecture. Morphometric parameters are extracted by automated image processing, and used to quantify the degree of pathological alterations. This offers unique potential to extend histology and pathohistology to study e.g. SARS-CoV-2 infected tissue or other lung degrading diseases such as COPD or cystic fibrosis, as we show with first applications of the method.

BP 21.10 Thu 12:15 BAR Schö

Dynamic allometry of nuclei and cell size in early embryos of a model organism — Rolf Fickentscher[1], Tomoko Ozawa[2], Akatsuki Kimura[2], and •Matthias Weiss[1] — [1]Experimental Physics I, University of Bayreuth, Germany — [2]Cell Architecture Laboratory, National Institute of Genetics, Mishima, Japan

Allometric relations between two observables are a widespread phenomenon in biology. The volume of nuclei, for example, has frequently been reported to be linearly related to the cell volume, but also conflicting, sublinear power-law correlations have been reported. Given that nuclei are vital organelles that harbor and maintain the cells' DNA, an understanding of the allometric scaling of nuclear volumes, which eventually defines the concentration and accessibility of chromatin, is of high interest. Using the model organism Caenorhabditis elegans, we show here that the allometry between cell and nucleus volumes is a dynamically adapting phenomenon with an asymptotic linear scaling. The adaption rate of the nucleus volume also scales with cell size. Our experimental data are well captured by a simple and supposedly generic model based on a diffusion-limited liberation of chromatin sites which drives decompaction and hence nucleus growth. Extrapolating our results to the general case of growing and proliferating cells suggests an isometric scaling of cell and nucleus volumes as the generic case.

BP 21.11 Thu 12:30 BAR Schö

Mechanical and electrophysiological recordings of neural organoids — Elijah Shelton[1], Paulina Wysmolek[2], Filippo Kiessler[1], Achim Brinkop[1], Sebastian Willenberg[1], Michael Frischmann[1], and •Friedhelm Serwane[1,2,3] — [1]Faculty of Physics & CeNS, LMU Munich, Germany — [2]MPI for Medical Research, Heidelberg, Germany — [3]Munich Cluster for Systems Neurology, Munich, Germany

Stem-cell derived organoids have made the exploration of neuronal network function accessible in vitro and are now allowing disease modelling. Both biochemical and mechanical signals, such as the elastic modulus, modulate the underlying behaviour of neurons to connect to networks. My group is developing tools for the mechanical and electrophysiological characterization of neuronal organoids. I will present a minimal-complexity setup for 3D imaging of their network activity

(Wysmolek et al., Sci Rep 12, 20420, 2022). To extract Ca-signals we combine a lightsheet microscope as an add-on to a standard inverted microscope with computational tools. We created a 3D connectivity map by imaging spontaneous activity. As a next step, we apply statistical models to characterize the network behaviour. Changes in the tissue mechanical properties are one biophysical hallmark of tumour formation *in vivo*. We map the mechanical properties of tumor-forming cerebral organoids using ferrofluid droplets as mechanical actuators. Our measurements performed in neural organoids could inform researchers about the interaction between mechanics and function in the central nervous system.

BP 21.12 Thu 12:45 BAR Schö

Multi-scale X-Ray phase contrast tomography from the whole cochlea to single cells — •Jannis Justus Schaeper[1], Christoph Kampshoff[2], Bettina Wolf[2], Daniel Keppeler[2], Tobias Moser[2], and Tim Salditt[1] — [1]Institut für Röntgenphysik, Georg-August-Universität Göttingen — [2]InnerEarLab, Universitätsmedizin Göttingen

The cochlea is the receptor organ of the inner ear which transduces sound into neuronal activity. Both fundamental aspects of signal transduction and neuro-physiology as well as biomedical research (implant technology, hearing loss and disorders) require 3D imaging techniques capable to quantify the micro-anatomy (1).

We present multi-scale 3D imaging of small-animal cochleae by X-ray phase-contrast tomography (XPCT) using both synchrotron radiation (SR) and lab μ-CT to assess the morphology of the cochlea, orientation of cochlear implants (CIs), and the number and density of spiral ganglion neurons (SGNs). Due to optimization in sample preparation, image acquisition and phase retrieval we achieve high contrast for unstained soft tissue. Without extensive sample preparation, shape and volume of every SGN in the entire organ can be identified. In the high-resolution PC-CT, and in the parallel beam, we reach cellular resolution in the organ of Corti. Lab μ-CT is suitable to analyze cochlear morphology and to assess the correct positioning of CIs and resulting (non-)optimal signal transduction.

(1) Keppeler et al. (2021), PNAS 118(18), e2014472118 (2) Schaeper et al. (2022), Proc. SPIE 12242

BP 22: Statistical Physics of Biological Systems I (joint session BP/DY)

Time: Thursday 9:30–13:00 Location: TOE 317

BP 22.1 Thu 9:30 TOE 317

Reduced stochastic models of drifting assemblies in plastic neuronal networks — •Sven Goedeke, Christian Klos, Yaroslav Felipe Kalle Kossio, and Raoul-Martin Memmesheimer — University of Bonn, Bonn, Germany

In a standard model, associative memories are represented by assemblies of strongly interconnected neurons. It has recently been proposed that these assemblies are not static but drift freely in neural circuits. On the level of single neurons, assembly drift is reflected by characteristic dynamics: relatively long times of stable assembly membership interspersed with fast transitions. How can we mechanistically understand these dynamics? Here we answer this question by proposing simplified, reduced models. We first construct a random walk model for neuron transitions between assemblies based on the statistics of synaptic weight changes measured in simulations of spiking neural networks exhibiting assembly drift. It shows that neuron transitions between assemblies can be understood as noise-activated switching between metastable states. The random walk's potential landscape and inhomogeneous noise strength induce metastability and thus support assembly maintenance in the presence of ongoing fluctuations. In a second step, we derive an effective random walk model from first principles. In this model, a neuron spikes at a fixed background rate and with an input weight-dependent probability when its current or another assembly reactivates. The approach can be applied generally to networks of drifting assemblies, irrespective of the employed neuron and plasticity models.

BP 22.2 Thu 9:45 TOE 317

Fluctuation-dissipation relations for spiking neurons — •Benjamin Lindner — Bernstein Center for Computational Neuroscience Berlin, Philippstr. 13, Haus 2, 10115 Berlin, Germany — Physics Department of Humboldt University Berlin, Newtonstr. 15, 12489 Berlin, Germany

Spontaneous fluctuations and stimulus response are essential features of neural functioning but how they are connected is poorly understood. I derive fluctuation-dissipation relations (FDR) between the spontaneous spike and voltage correlations and the firing rate susceptibility for i) the leaky integrate-and-fire (IF) model with white noise; ii) an IF model with arbitrary voltage dependence, an adaptation current, and correlated noise. The FDRs can be used to derive thus far unknown statistics analytically [model (i)] or the otherwise inaccessible intrinsic noise statistics [model (ii)].

BP 22.3 Thu 10:00 TOE 317

Current fluctuations in nanopores: origin and breakdown of 1/f noise — •Paul Robin, Mathieu Lizee, Alessandro Siria, and Lydéric Bocquet — ENS, Université PSL, CNRS, Sorbonne Université, Université Paris-Cité, Paris, France

Ion transport through nanometric pores is key to many biological processes, from osmoregulation to neurotransmission, yet this process is known to occur under strong fluctuations. The power spectrum of this current noise is known to scale like 1/f at low frequency, according to the long-standing yet empirical Hooge law. Modelling attempts generally rely on complex assumptions such as self-organized criticality or microscopic disorder - in contrast with the apparent universality of 1/f pink noise. In this talk, I will present a simple theoretical model accounting for the presence of 1/f fluctuations in ionic currents through nanopores regardless of their microscopic structure. In particular, I will show how pink noise can emerge from diffusive processes alone, rather than necessitating complex conductance switching mechanisms. This prediction also explains why pink noise can be observed for frequencies much lower than that of microscopic processes. Lastly, I will discuss under which conditions this description is expected to break down. Notably, chemical processes on the pore's walls can alter ion dynamics and slow down diffusion, leading to memory effects and deviations to Hooge's law. I will compare these predictions to experimental data on artificial nanofluidic pores with various surface properties and reactivities.

BP 22.4 Thu 10:15 TOE 317

Selective alignment force in schooling fish linked to leader-follower interactions given by relative speeds of neighbours — •Andreu Puy[1], Palina Bartashevich[2,3], and Pawel Romanczuk[2,3] — [1]Departament de Física, Universitat Politècnica de Catalunya, Barcelona, Spain — [2]Institute for Theoretical Biology, Humboldt-Universität zu Berlin, Germany — [3]Excellence Cluster Science of Intelligence, Technische Universität Berlin, Germany

Collective motion is commonly assumed to emerge when individuals in a group interact with neighbours via some combination of attraction, repulsion and alignment forces. Alignment has been the most elusive and controversial force to study in experimental setups, with previous works differing about its existence. Here we revisit the topic by introducing a force map technique depending on the relative velocities of neighbours. In contrast to commonly used force maps, our technique demonstrates evidence for experimental data of schooling fish of a selective alignment force when individuals move at slower speeds than their neighbours and an antialignment force when they move at higher speeds. We employ a simple model with alignment to demonstrate the validity and robustness of the proposed force map. Including a selective interaction where individuals only interact with faster neighbours allowed us to reproduce the alignment interactions in the experimental data. Finally, we link this idea to leader-follower interactions, justifying that faster individuals act as leaders with respect to their neighbours.

Invited Talk BP 22.5 Thu 10:30 TOE 317

Statistical Physics of Spatially Organized Catalytic Particles — •Ulrich Gerland — Technical University of Munich, Germany

Catalytic particles are spatially organized in a number of biological systems across different length scales, from enzyme complexes to metabolically coupled cells. Despite operating on different scales, these sys-

tems all feature localized reactions involving partially hindered diffusive transport, which is determined by the collective arrangement of the catalysts. We explore how different arrangements affect the interplay between the reaction and transport dynamics, which ultimately determines the flux through the reaction pathway. Two fundamental trade-offs arise, the first between efficient inter-catalyst transport and the depletion of substrate, and the second between steric confinement of intermediate products and the accessibility of catalysts to substrate. We find that the question of optimal catalyst arrangements generalizes the well-known Thomson problem of electrostatics [1]. Furthermore, we map the problem of optimally arranging enzymes to an economic investment problem, which helps to formulate and understand a possible design principle for synthetic biomolecular systems [2].

[1] F. Hinzpeter, F. Tostevin, A. Buchner, and U. Gerland (2022), Trade-offs and design principles in the spatial organization of catalytic particles, Nature Phys. 18, 203-211.

[2] G. Giunta, F. Tostevin, S. Tanase-Nicola, and U. Gerland (2022), Optimal spatial allocation of enzymes as an investment problem, Commun. Phys. 5, 319.

15 min. break

BP 22.6 Thu 11:15 TOE 317

Collective Dynamics of Multi-Scale Interacting Complex Systems — •Fabrizio Olmeda[1,2] and Steffen Rulands[1,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]IST Austria, Vienna, Austria — [3]Ludwigs-Maximilians-Universitat Munchen, Arnold Sommerfeld Center for Theoretical Physics, Munich, Germany

Understanding the conditions under which complex systems are stable is pivotal for understanding their response to perturbations. Theoretical work has shown that for global interactions between components a minimal complex system is stable if the standard deviation of linearised interaction rates is sufficiently small. In biological systems, which often contain a small number of important and interactions are mediated by diffusing agents, stochasticity and non-locality may influence stability. Here, we generalise these results to stochastic, spatial systems with interaction on multiple length scales. Starting from a microscopic description we derive a coarse-grained field theory and identify a transition between a regime defined by giant density fluctuations and one exhibiting a spatial instability with a finite wave length. The latter is suppressed by non-reciprocity in the interactions between components. Our work provides a rigorous framework to infer collective dynamics and stability in complex systems, with applications ranging from ecosystems to morphogenesis.

BP 22.7 Thu 11:30 TOE 317

Physical mechanism of erythrocytes sedimentation rate — •Alexis Darras, Thomas John, Lars Kaestner, and Christian Wagner — Experimental Physics, Saarland University; D-66123 Saarbrücken, Germany

Red blood cells (or erythrocytes) sedimentation rate (ESR) is a physical parameter of blood which is often checked in medical diagnosis. It is indeed well known that in case of inflammation, the increase in fibrinogen and other proteins induces a higher ESR.

Until recently, researchers thought that the increase of fibrinogen accelerates the ESR by creating bigger aggregates of red blood cells (RBC). Fibrinogen is indeed an aggregation agent of RBCs, and bigger aggregates tend to sediment faster in Stokes regime. However, modeling the ESR measurements with this hypothesis is challenging and often requires physical assumptions specific to this system.

Besides, modern colloidal science has shown that attractive particles, in suspensions with a high volume fraction, form percolating aggregates, as wide as the container. The sedimentation of those colloids then follows a so-called "colloidal gel collapse" regime, governed by the geometry of the percolating aggregate acting as a porous material. In this talk, we show that RBCs actually follow the same behavior. We also demonstrate that a porous-material model naturally leads to an efficient description the RBC sedimentation, which also provides a long-sought dependency of the ESR as a function of the initial RBC volume fraction (i.e. the hematocrit).

BP 22.8 Thu 11:45 TOE 317

Stochastic wavelength selection and pattern fixation — •Tom Burkart[1,2], Anastasiia Petrova[2,3], Laeschkir Würthner[1,2], Claudia Veigel[2,3], and Erwin Frey[1,2,4] — [1]Arnold Sommerfeld Center for Theoretical Physics (ASC), Department of Physics, LMU München, Munich, Germany — [2]Center for NanoScience, LMU München, Munich, Germany — [3]Department of Cellular Physiology, Biomedical Center (BMC), LMU München, Planegg-Martinsried, Germany — [4]Max Planck School Matter to Life, Munich, Germany

Biological pattern-forming processes are typically driven by a chemical fuel (out-of-equilibrium systems) or by a relaxation towards a thermodynamic equilibrium (phase separation). In these cases, pattern wavelength selection results from translational shifts of high-density regions and mass redistribution in between such regions. Here, we study how a pattern with a characteristic wavelength can form when high-density regions can only grow, but neither mass redistribution nor translation are allowed. The corresponding wavelength selection mechanism relies on thermal fluctuations, irreversible fixation of randomly occurring high-density regions, and long-ranged interactions between these regions. To model the density dynamics and the long-ranged interaction, we derive a set of reaction-diffusion equations from a free energy functional. In addition, we derive the statistics of pattern wavelengths from order statistics, emphasising the stochastic nature of the underlying mechanism. Our results constitute an alternative path to pattern formation next to out-of-equilibrium dynamics and phase separation processes.

BP 22.9 Thu 12:00 TOE 317

Control of non-equilibrium chemical reactions via phase separation — •Sudarshana Laha[1,2], Jonathan Bauermann[1,2], Tyler S. Harmon[3], Frank Jülicher[1,2], Thomas C.T. Michaels[4], and Christoph A. Weber[5] — [1]Max Planck Institute for the Physics of Complex Systems Dresden , Germany — [2]Center for Systems Biology Dresden , Germany — [3]IFW Dresden, Germany — [4]ETH Zürich, Switzerland — [5]Institute of Physics, University of Augsburg, Germany

Fuel-driven out-of-equilibrium chemical reactions are spatially organized using compartments in living cells. To what extent the properties of chemical reactions are altered by the compartments relative to homogeneous systems and the underlying physical principles are less explored. Here, we derive a theoretical framework to study such chemical reactions in the presence of compartments. We highlight the different governing kinetic equations for the reactants in diffusion-limited and reaction-limited regimes. We show that for two-state transition processes, the turnover of the product can be significantly affected in the limit of infinitely fast diffusion of the components. We can further derive the optimal compartment volume analytically which shows how phase separation parameters can affect the turnover. We further observe that the initial rate can be strongly modified for enzymatic and nucleation processes. These aspects allow us to understand better the control of such processes and exemplify the role of enzymes in compartments to speed up the reaction. This understanding is crucial for synthetically designing of cells as compartments and establishing communication between them.

BP 22.10 Thu 12:15 TOE 317

Microphase separation of living cells — •François Detcheverry, Adrien Carrère, Joseph d'Alessandro, Olivier Cochet-Escartin, Julie Hesnard, Nasser Ghazi, Charlotte Rivière, Christophe Anjard, and Jean-Paul Rieu — University of Lyon, Université Claude Bernard Lyon 1, CNRS, Institut Lumière Matière, F-69622, VILLEURBANNE, France

Self-organization of cells is key to a variety of biological systems and physical concepts inspired from condensed matter have proven essential in understanding some of their properties. Here we demonstrate that microphase separation, long known in polymeric materials and other inert systems, has a natural counterpart in living cells. When placed below a millimetric film of liquid nutritive medium, a quasi two-dimensional population of *Dictyostelium discoideum* cells spontaneously self-assembles into compact domains. Their typical size of 100 μm is governed by a balance between competing interactions: an adhesion which acts as a short-range attraction and promotes aggregation, and an effective long-range repulsion stemming from aerotaxis in near anoxic condition. We present a combination of experimental data, analytical modelling and cell-based simulations that all support this scenario. Our findings establish a generic mechanism for self-organization of living cells and highlight oxygen regulation as an emergent organizing principle for biological matter.

[Preprint: bioRxiv https://doi.org/10.1101/2022.05.25.493184]

BP 22.11 Thu 12:30 TOE 317

Hydrationa and crowding effects on SOD1 sequestration

into FUS biocondensates — Luis Enrique Coronas[1], Emeline Laborie[2], Stepan Timr[2], Fabio Sterpone[2], and •Giancarlo Franzese[1,3] — [1]Interdisciplinary and Statistical Physics Section–Department of Condensed Matter Physics, Physics & Institute of Nanoscience and Nanotechnology (IN2UB), Universitat de Barcelona, Barcelona, Spain — [2]CNRS Laboratoire de Biochimie Théorique, Institut de Biologie Physico-Chimique, Université Paris Denis Diderot, Paris, France — [3]Max Planck Institut für Physik Komplexer Systeme, Dresden, Germany

Superoxide Dismutase 1 (SOD1) is a protein related to amyotrophic lateral sclerosis that, under Heat Stress (HS), is sequestered into Stress Granules in vivo and Fused in Sarcoma (FUS) biomolecular condensates in vitro. Experiments show that an in vitro cytomimetic medium, using Bovine Serum Albumin (BSA) as crowder, decreases the SOD1 partition coefficient (PC) even after 60 min of HS. Implicit-water OPEP simulations show no preferential interactions of SOD1 with BSA. Here, by combining the OPEP with a coarse-grained water model, accounting for water contributions to the interactions in large biological systems, we show that SOD1 has one preferred associative state in FUS but three in BSA, whose transition rates and residency times are controlled by their hydration. We conclude that the SOD1 PC's decrease in FUS condensate, when BSA crowders are present, is due to the hydration entropy increase in BSA, a mechanism possibly relevant also in vivo.

BP 22.12 Thu 12:45 TOE 317

Stochastic heat production in phase-separated systems out of equilibrium — •Kathrin Laxhuber, Jonathan Bauermann, and Frank Jülicher — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Phase-separated multi-component systems in the presence of chemical reactions provide interesting examples of non-equilibrium systems. We complement the dynamics of phase separation by a heat transport equation which is coupled to diffusive matter transport. On a microscopic scale, fluctuations become relevant, which we include by developing a stochastic lattice model that we link to the macroscopic continuum dynamics. We then implement this model in a kinetic Monte Carlo simulation of spatial flows of energy and matter as well as local reactions. By coupling to reservoirs or by fueling reactions, a system can be driven out of equilibrium. Using a toy system of a single phase-separated droplet, we discuss how temperature fluctuations affect the droplets' dynamics and the noise in the system. We furthermore show how the fluxes due to the driving give rise to a stochastic production of latent heat and reaction heat. The systems we discuss serve as models for biological condensates and the study of energetics in cells.

BP 23: Single Molecule Biophysics

Time: Thursday 9:30–13:00 Location: BAR 0106

Invited Talk BP 23.1 Thu 9:30 BAR 0106

Conformational dynamics of SARS-CoV-2 spike protein modulates the binding affinity to ACE2 — Fidan Sumbul[1], Claire Valotteau[1], Prithwidip Saha[1], Ignacio Fernadez[2], Annalisa Meola[2], Eduard Baquero[2], Dorota Kostrz[3], James R Portman[3], François Stransky[3], Pablo Guardado Calvo[2], Charlie Gosse[3], Terence Strick[3], Felix Rey[2], and •Felix Rico[1] — [1]Aix-Marseille Univ, CNRS, INSERM, LAI, CENTURI, Marseille, France — [2]Institut Pasteur, Department of Virology, CNRS UMR 3569, Paris France — [3]Ecole Normale Superieure, Institut de Biologie, CNRS, INSERM, PSL, Paris, France

SARS-CoV-2 spike protein (S) interacts with angiotensin-converting enzyme 2 (ACE2) to enter host cells. Protein S forms a homotrimer with three receptor-binding domains (RBD) adopting open and closed conformations. The (un)binding of S to ACE2 may be affected by these conformational dynamics. Here, we used single molecule force spectroscopy to probe the binding strength and affinity of the S-trimer/ACE2 interaction and high-speed atomic force microscopy (HS-AFM) to visualize the RBD opening dynamics of S-trimers. HS-AFM imaging revealed dynamic S-trimers with the three RBDs stochastically and independently switching between open and closed conformations. This modulates binding to ACE2 of S-trimers, but not unbinding. Experimental opening rates and a simple conformational binding model explain the modulation of the binding affinity. Our results shed light on the molecular basis of coronavirus infection.

BP 23.2 Thu 10:00 BAR 0106

ion-specific DNA adsorption at mica mediated by monovalent and divalent metal cations — •Ibrahim Mohd[1], Max Lallemang[2], Bizan N Balzer[2], and Ibrahim Mohd[1] — [1]University of Augsburg, 86159 Augsburg, Germany — [2]universitätsstraße 1

Ion mediated attraction between biomolecules and solid substrates plays a crucial role in a broad range of biotechnological applications. In this work, we combine molecular dynamics simulations and single-molecule atomic force microscopy experiments to characterise the desorption properties of single-stranded DNA at mica surface mediated by the alkali and alkaline earth metal ions Li+, Na+, K+, Cs+, Mg2+ and Ca2+. Our results show that both monovalent and divalent ions induce an attractive interaction between DNA and the negatively charged mica surface. DNA adhesion is caused by two effects: Firstly, ion-specific adsorption of the monovalent cations compensates the negative charge and induces a long-ranged attraction. In addition, the surface adsorbed cations form inner-sphere contacts with the oxygen atoms of the DNA backbone. Both effects depend on the type of cation: Cs+ and K+ ions lead to loosely associated DNA with high surface mobility and low rupture forces. Na+, Li+, and divalent ions lead to a stronger association of DNA with low surface mobility and high rupture forces. By comparing the force-extension curve shapes from experiments and simulations we could provide atomistic insights into the desorption mechanisms and identify the dominant interactions involved in the desorption process.

BP 23.3 Thu 10:15 BAR 0106

Understanding the molecular determinants of chitin-protein interactions in the arthropod cuticle - a single-molecule approach — •Ayesha Talib[1,2], Yael Politi[2], and Kerstin G. Blank[1,3] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]Technische Universität Dresden, CMCB, B CUBE, Dresden, Germany — [3]Johannes Kepler Universität, Institute of Experimental Physics, Linz, Austria

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

BP 23.4 Thu 10:30 BAR 0106

Complex unfolding, refolding and DNA association of the relaxase TrwC — •César Augusto Quintana-Cataño[1], •Miriam Schramm[1], Ekaterina Vorobevskaia[1], Andreas Hartmann[1], and Michael Schlierf[1,2] — [1]B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany — [2]Cluster of Excellence Physics of Life, TU Dresden, Germany

Referred as "bacterial sex", bacterial conjugation is a process in which a donor cell transfers DNA to a recipient cell. Conjugation is a main driver for spreading of antibiotic resistance genes. The relaxase TrwC associated to the type 4 secretion system is a multi-domain model enzyme essential for bacterial conjugation. It serves multiple purposes: DNA recognition, nicking and unwinding in the donor cell; and re-

ligation of ssDNA in the receptor cell. For this last step a mechanical unfoldase denaturates TrwC, which then refolds in the receptor cell. TrwC is a multi-domain protein consisting of 966 amino acids with a 55 amino acids long intrinsically disordered C-terminus. Here, we studied unfolding and folding mechanics of TrwC using single-molecule magnetic tweezers force spectroscopy. We show that the subdomains of TrwC unfold at distinct, different force regimes ranging from ˜10 pN to 90 pN and TrwC refolds in a complex multistep reaction. Using our data, we can quantify the folding energetics of TrwC. We have further discovered complex DNA binding events of monomers and dimers using fluorescence correlation spectroscopy, allowing us to build a model of DNA association. We anticipate that our data helps to understand a key enzyme of DNA conjugation and its multifold activities.

BP 23.5 Thu 10:45 BAR 0106

Superpower behavior of the budding yeast kinesin-8 — •Anita Jannasch, Brent Fielden, Michael Bugiel, and Erik Schäffer — Universität Tübingen

Kinesin-8 motor proteins can regulate microtubule dynamics and their length. Furthermore, they can crosslink microtubules and slide them relative to each other. These properties make the motor important for cell division. The budding yeast kinesin-8, Kip3, depolymerizes microtubule in a collective, force and length-dependent manner. The latter is due to the motor's very high processivity. Recently, we found that contrary to the depolymerization activity of multiple motors, a single Kip3 motor stabilizes microtubules. Compared to conventional kinesin, Kip3 is more than 10x slower and can generate about a 5x lower maximum force suggesting that it is a low power motor. Surprisingly, using high-precision optical tweezers, we observed that single Kip3 bound via a nanobody to optically trapped microspheres occasionally moved about 6x faster generating 3x higher forces compared to its usual behavior. This superpower behavior is almost comparable to conventional kinesin, but it is unclear whether it is related to one of its biological functions. The nanobody coupling also reduced the compliance of the system and thereby improved the spatiotemporal resolution. With the improved resolution, we were able to detect 4-nm mechanical substeps of the motor. In the long term, a better understanding of the various talents of Kip3 on the molecular level will have implications for cell division and associated diseases.

BP 23.6 Thu 11:00 BAR 0106

Thermodynamic inference for molecular motor models based on non-invasive conditioned waiting-time measurements — •Benjamin Ertel, Jann van der Meer, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Molecular motors are one example of biophysical systems operating far from equilibrium. For the description of their dynamics in motor-bead assays, three classes of models have been proposed. The first class, discrete Markov networks, emphasizes the configurational changes of the motor where the bead enters the transition rates. The second class of models focuses on the motion of the bead, which is described by an overdamped Langevin equation. The third class of models, hybrid motor-bead complexes, describes the full dynamics of the motor-bead assay by combining discrete and continuous models from the two previous classes. In this work, we develop a thermodynamic inference scheme that can be used to distinguish qualitatively between the different classes of models. Since this inference scheme is based on the observation of waiting times for conditioned transitions of the bead trajectory only, it is non-invasive and operationally accessible in experiments. Various characteristics of the motor, like its driving affinity, can be inferred without further information. We have obtained these results through analytical derivations and extensive numerical calculations.

15 min. break

BP 23.7 Thu 11:30 BAR 0106

Metal-protein-metal junctions: electron transport and mechanical deformation — •Linda Angela Zotti — Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain

Proteins have proven to be promising candidates for molecular electronics, showing in some cases much higher conductance than one would naively expect from their size. In particular, the blue-copper azurin extracted from Pseudomonas aeruginosa has been the subject of many experimental studies, although the exact electron-transport mechanism is still under debate. Here I will present our efforts towards understanding the origin of such interesting effects from a theoretical perspective, analyzing both the electronic structure and the geometrical arrangement [1-6].

References [1] M. P. Ruiz et al. , J. Am. Chem. Soc. 139, 43, 15337 (2017). [2] C. Romero Muñiz, M. Ortega, J.G Vilhena, I. Diéz Pérez, R. Pérez, J. C. Cuevas, L. A. Zotti, Phys. Chem. Chem. Phys., 20, 30392 (2018). [3] C. Romero Muñiz, M. Ortega, J.G Vilhena, I. Diéz Pérez, R. Pérez, J. C. Cuevas, L. A. Zotti, Biomolecules, 9(9), 506 (2019). [4] C. Romero Muñiz, M. Ortega, J.G Vilhena, I. Diéz Pérez, R. Pérez, J. C. Cuevas, L. A. Zotti, J.Phys.Chem.C 125 (3), 1693 (2021). [5] C. Romero Muñiz, M. Ortega, J.G Vilhena, R. Pérez, J. C. Cuevas, L. A. Zotti, Appl. Sci. 11 (9), 3732 (2021). [6]C. Romero Muñiz, J.G Vilhena, R. Pérez, J. C. Cuevas, L. A. Zotti, Front. Phys. 10:950929. doi: 10.3389/fphy.2022.950929 (2022).

BP 23.8 Thu 11:45 BAR 0106

A variance sum rule and its entropy production estimation — •Ivan Di Terlizzi[1,2], Marta Gironella[3], Marco Baiesi[3], and Felix Ritort[2] — [1]Max Planck Institute for the Physocxs of complex systems — [2]University of Padua — [3]University of Barcelona

Nonequilibrium steady states, from the planetary scale to biological processes, are characterized by entropy production via energy dissipation to the environment, which is often challenging to measure. A novel variance sum rule sets a new resource for exploiting fluctuations to measure physical quantities in stochastic systems. In particular, we focus on the formula it gives for estimating the entropy production rate from trajectories of positions and forces. We describe this method with analytically solvable models and we show its robustness and usefulness in practical applications to experimental data. By introducing a model-dependent fitting procedure, the method is also adapted to deal with conditions where not all degrees of freedom are experimentally accessible. For example, by analysing traces of flickering red blood cells, we obtain estimates of the entropy production rate in line with values obtained with totally different thermodynamic techniques.

BP 23.9 Thu 12:00 BAR 0106

Lattice defect sites accelerate microtubule severing by spastin — •Cordula Reuther[1], Paula Santos-Otte[1], Rahul Grover[1], and Stefan Diez[1,2,3] — [1]B CUBE - Center for Molecular Bioengineering, TU Dresden, Dresden, Germany — [2]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany — [3]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Length regulation of microtubules and their organization into complex arrays occurs through the activity of polymerases, depolymerases as well as severing enzymes such as katanin and spastin. The latter hexamerize on the microtubule lattice, pull out single tubulin dimers in an ATP-dependent manner and eventually generate internal breaks in the microtubule. For both enzymes it was shown that the severing activity is regulated by tubulin posttranslational modifications. So far, however, only katanin has been reported to exhibit a lattice-defect- or crossover-sensing activity. Here, we determined whether lattice defects in GMPCPP-stabilized microtubules also affect the severing activity by spastin. In controlled in vitro assays we characterized microtubules with defects next to control microtubules. Defect sites were introduced either through specific polymerization conditions or by end-to-end annealing of microtubules. We found that (i) the presence of defects accelerated the onset of the severing process and (ii) severing occured twice as often in microtubule segments with defect sites as compared to random lattice segments. Furthermore, we quantified the correlation of the fluorescence signal of GFP-labelled spastin along the microtubule lattice to the severing sites as a function of time.

BP 23.10 Thu 12:15 BAR 0106

Keratin filament mechanics and energy dissipation are determined by metal-like plasticity — •Charlotta Lorenz[1], Johanna Forsting[1], Robert W. Style[2], Stefan Klumpp[3], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Department of Materials, ETH Zürich, Vladimir-Prelog-Weg 1-5/10, 8093 Zürich, Switzerland — [3]Institute for the Dynamics of Complex Systems, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Cell mechanics is determined by an intracellular biopolymer network, including intermediate filaments that are expressed in a cell-type specific manner. A prominent pair of intermediate filaments are keratin

and vimentin as the epithelial-to-mesenchymal transition is associated with a switch from keratin to vimentin. The transition coincides with a change in cellular mechanics, and thus dynamic properties of the cells. This observation raises the question of how the mechanical properties already differ on the single filament level. Here we use optical tweezers and a computational model to compare the stretching and dissipation behavior of the two filament types. We find that keratin and vimentin filaments behave in opposite ways: keratin filaments elongate, but retain their stiffness, whereas vimentin filaments soften, but retain their length. This finding is explained by fundamentally different ways to dissipate energy: viscous subunits sliding within keratin filaments and non-equilibrium α helix unfolding in vimentin filaments.

BP 23.11 Thu 12:30 BAR 0106

The single-strand annealing protein RAD52 can form a stable nucleoprotein filament — •Carolina Carrasco[1], Laura Muras[1], Tobias Jachowski[1], Sivaraman Subramaniam[2], Francis Stewart[2], and Erik Schäffer[1] — [1]Center for Plant Molecular Biology (ZMBP), University of Tübingen, Tübingen, Germany — [2]Department of Genomics, Biotechnology Center, TU Dresden, Dresden, Germany

Genome maintenance requires the repair of DNA double-strand breaks. It can be mediated among others by the single-strand annealing. RAD52 proteins form rings that are thought to promote the annealing. How RAD52 interacts with and anneals DNA strands remains unclear. We have investigated the dynamic interaction of RAD52 with DNA by force spectroscopy using optical tweezers. Upon stretching single DNA molecules in the presence of RAD52, we have observed elongation steps in DNA extension that are consistent with either dissociation, unwrapping, or opening of individual DNA-bound rings. Upon relaxation, reverse steps of similar amplitude were detected. Under constant force, step sizes were uniform. Surprisingly, the disruption forces followed a gamma distribution suggesting that the RAD52-DNA dissociation process consists of multiple stochastic steps. Successive stretch-relax cycles at high forces promoted DNA softening and a melting-force increase because of an intercalation and sealing mechanism on DNA. The final DNA-RAD52 hysteresis-free nucleoprotein filament is consistent with a flexible helical structure in which RAD52 monomers, and not rings, mediate strand annealing.

BP 23.12 Thu 12:45 BAR 0106

Assessing biomolecular interactions across scales using optical tweezers — •Roman Renger, Nicholas Luzzietti, and Philipp Rauch — Paalbergweg 3, 1105 AG Amsterdam, Netherlands

Biological processes involving proteins interacting with nucleic acids, cell membranes or cytoskeletal filaments are key to cell metabolism and hence to life in general. Detailed insights into these processes provide essential information for understanding the molecular basis of physiology and the pathological conditions that develop when such processes go awry. The next scientific breakthrough consists in the direct, real-time observations and measurements of the most fundamental mechanisms involved in biology Single-molecule technologies offer a powerful opportunity to meet these challenges and to study dynamic protein function and activity in real-time and at the single-molecule level. Here, we present our efforts for further enabling discoveries in the field of biology and biophysics using the combination of optical tweezers with correlative fluorescence microscopy (widefield, TIRF, confocal and STED) and label-free Interference Reflection Microscopy (IRM). We present several examples in which our technology has enhanced the understanding of basic biological phenomena, ranging from protein structure to intracellular organization. Furthermore, we show that advances in hybrid single-molecule methods can be turned into an easy-to-use and stable instrument that has the ability to open up new avenues in many research areas.

BP 24: Active Matter IV (joint session DY/BP/CPP)

Time: Thursday 9:30–13:00 Location: ZEU 160

Invited Talk BP 24.1 Thu 9:30 ZEU 160

Acoustically propelled nano- and microparticles: From fundamentals to applications — •Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Among the existing types of artificial active colloidal particles, acoustically propelled nano- and microparticles have a particularly high potential for future applications in fields like medicine and materials science. However, despite intensive research on this type of motile particles in recent years, the understanding of their properties is still very limited. A reason for the limited understanding is that the previous research has mostly been experimental and that it is difficult to study the dependence of certain system parameters on the propulsion of the particles in experiments since the parameters can often not be varied independently of the other parameters and in ranges of reasonable size. In this talk, I will give an overview about our theoretical investigation of the properties of acoustically propelled nano- and microparticles and the challenges that remain for future research.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – 283183152 (WI 4170/3).

BP 24.2 Thu 10:00 ZEU 160

Force on probe in a confined active fluid — Shuvojit Paul[1], •Ashreya Jayaram[2], N Narinder[1], Thomas Speck[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, 78464 Konstanz, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany

When immersed in a dispersion of smaller "depletants", a colloidal particle experiences depletion forces in the presence of another colloidal particle or under confinement. While the nature of these forces is well-established for passive systems, much less is known about the consequence of making the depletants self-propelled or "active". In this work, we consider a large, optically trapped probe under circular confinement surrounded by smaller active Janus particles. We find that the force experienced by the probe varies non-monotonically as the distance between the colloid and the confinement is increased. To rationalize this observation, we relate the measured force to the active stress and, subsequently, to the microstructure of the surrounding active fluid. Going beyond synthetic active matter, our work could shed light on the organization of intracellular entities in biological systems.

BP 24.3 Thu 10:15 ZEU 160

Symmetry-breaking refractive index profiles as a propulsion mechanism for active Brownian particles — •Julian Jeggle[1], Matthias Rüschenbaum[2], Cornelia Denz[2], and Raphael Wittkowski[1] — [1]Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Institut für Angewandte Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Active Brownian particles (ABPs) have been realized with various propulsion mechanisms such as self-diffusiophoresis, self-electrophoresis or acoustic scattering. Typically, these mechanisms induce flow fields around the particles that represent a deviation from the "pure" ABP model. Here, we present a novel implementation of ABPs in the form of transparent microswimmers with a symmetry-breaking refractive index gradient. Utilizing the momentum transfer associated with light refraction as the driving force induces no flow fields beyond Stokes flow. Unlike optothermally driven particles, this archetype of ABPs also allows for sensitivity to the phase and polarization of the driving light field thus improving the spatio-temporal control of light-based propulsion mechanisms. Using non-light-absorbing particles enables bulk volume systems and allows the introduction of feedback loops, therefore making this approach a promising foundation for adaptive matter systems.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – Project-ID 433682494 - SFB 1459

BP 24.4 Thu 10:30 ZEU 160

The interaction-expansion method: a systematic derivation strategy for active field theories* — •Michael te Vrugt[1,2], Jens Bickmann[1,2], Stephan Bröker[1,2], Tobias Frohoff-Hülsmann[1], Eyal Heifetz[3], Michael E. Cates[4], Uwe Thiele[1,5,6], and Raphael Wittkowski[1,2,5] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]SoN, Westfälische Wilhelms-Universität Mün-

ster — [3]Porter School of the Environment and Earth Sciences, Tel Aviv University, 69978 Tel Aviv, Israel — [4]DAMTP, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom — [5]CeNoS, Westfälische Wilhelms-Universität Münster — [6]CMTC, Westfälische Wilhelms-Universität Münster

Field-theoretical models have made enormous contributions to our understanding of the collective dynamics of active matter. In this contribution, we introduce the interaction-expansion method (IEM) [1], which allows for a systematic derivation of active field theories from the microscopic dynamics of individual particles. We then discuss some recent applications of the IEM to particles with orientation-dependent propulsion speed [2] and particles with inertia [3].

[1] M. te Vrugt et al., in preparation (2022)

[2] S. Bröker et al., arXiv:2210.13357 (2022)

[3] M. te Vrugt et al., Nature Communications (provisionally accepted), arXiv:2204.03018 (2022)

⋆ *Funded by the Deutsche Forschungsgemeinschaft (DFG)– 283183152*

BP 24.5 Thu 10:45 ZEU 160

Entropy production in active turbulence — •Byjesh Nalini Radhakrishnan, Thomas Schmidt, and Etienne Fodor — Department of physics and material science, University of Luxembourg

Active particles like bacteria and sperm cells sustain a continuous intake and dissipation of energy. Consequently, they are intrinsically out of equilibrium which leads to a non-vanishing entropy production rate (EPR) even in steady states. Quantifying how the EPR varies in different collective phases is crucial in developing a thermodynamic framework for active matter. In this work, we look at the EPR in active turbulence. We use Active Model H, a continuum model for active particles in a momentum-conserving fluid, to study turbulence in contractile scalar active systems. We measure the local EPR in numerical simulations, which unveils the role of the noise and activity parameters on the EPR in active turbulent systems.

15 min. break

BP 24.6 Thu 11:15 ZEU 160

Phase transitions in multicomponent active matter: a quantitative kinetic theory — •Jakob Mihatsch[1], Thomas Ihle[1], Rüdiger Kürsten[2], and Horst-Holger Boltz[1] — [1]Institute for Physics, University of Greifswald, Greifswald, Germany — [2]Departament de Física de la Matèria Condensada, University of Barcelona, Barcelona, Spain

We consider a multicomponent model of self-propelled particles with Kuramoto-type alignment interactions. Starting from the N-particle Fokker-Planck equation we observe that the usual factorization Ansatz of the probability density, often called Molecular Chaos approximation, predicts a relaxation behavior which qualitatively disagrees with agent-based simulations. Therefore, we develop a kinetic theory which takes the time-evolution of the two-particle correlation function explicitly into account, i.e. goes beyond the mean-field approximation. We show that this theory predicts the relaxation behavior of the system as well as the order-disorder transition with high precision in certain parameter ranges. In particular, the dependence of the transition threshold on the particle speed is predicted correctly.

BP 24.7 Thu 11:30 ZEU 160

Emergent collective behaviour due to virtual interactions between robotic swimmers — •Samudrajit Thapa[1,2], Bat-El Pinchasik[1,3], and Yair Shokef[1,2,3] — [1]School of Mechanical Engineering, Tel Aviv University, Tel Aviv 69978, Israel — [2]Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv 69978, Israel — [3]Center for the Physics and Chemistry of Living Systems, Tel Aviv University, 69978, Tel Aviv, Israel

Many organisms in nature use local interactions to realize global collective behaviour. Here we study how simple two body distance-based interactions between active Brownian particles results in collective motion. The interactions are not physical but virtual, wherein each particle senses the presence of other particles nearby and changes its behaviour accordingly. We study the radial distribution function to quantify the emergent interactions for both social and anti-social behaviour. Using Langevin dynamics simulations, we discover that under certain conditions positive correlations of the motion can emerge even in the case of anti-social behaviour. Our results might be potentially useful for designing robotic swimmers that can swim collectively just based on sensing the distance to their neighbours.

BP 24.8 Thu 11:45 ZEU 160

Kinetic Event-Chain Algorithm for Active Matter — •Nico Schaffrath, Thevashangar Sathiyanesan, Tobias Kampmann, and Jan Kierfeld — Physics Department, TU Dortmund University, 44221 Dortmund, Germany

We present a cluster kinetic Monte-Carlo algorithm for active matter systems of self-propelled hard particles. The kinetic event-chain algorithm is based on the event-chain Monte-Carlo method and is applied to active hard disks in two dimensions. The algorithm assigns Monte-Carlo moves of active disks a mean time based on the mean and variance of the move length in force direction. This time is used to perform diffusional rotation of their propulsion force. We show that the algorithm reproduces the motility induced phase separated region in the phase diagram of hard disks correctly and efficiently.

BP 24.9 Thu 12:00 ZEU 160

Emergent pattern formation in communicating active matter — •Robert Grossmann[1], Zahra Mokhtari[2], Robert I.A. Patterson[3], and Felix Höfling[2,4] — [1]Institut für Physik und Astronomie, Universität Potsdam — [2]Institut für Mathematik, Freie Universität Berlin — [3]WIAS Berlin — [4]Zuse Institut Berlin

Inspired by trail formation as observed in colonies of driver ants, for example, we study ensembles of agent particles that communicate via deposition and sensing of pheromones. These chemical traces are produced by the agents themselves and encode their current position and walking direction. Other agents passing by will then tend to align with the orientation inscribed in the pheromone traces. In the limit of short pheromone lifetime, the dynamics of this system reduces to the seminal Vicsek model and, thus, yields the formation of transversally moving bands. In the opposite limit, the effective agent-agent interaction represents a form of delayed feedback and yields the spontaneous formation of macroscopic, persistent trails, which are followed and reinforced by the agents [New J. Phys. **24** 013012 (2022)]. In this talk, we present large-scale simulations of the agent model and establish the phase diagram as function of the lifetime of pheromones. We rationalize our findings by analyzing mean-field equations that are systematically derived from the stochastic particle model. Combining numerical solutions of these order parameter equations and a linear stability analysis, we show how transversal bands, common in the Vicsek model, are destabilized, giving rise to the formation of "longitudinal" trails, pointing in the mean direction of motion.

BP 24.10 Thu 12:15 ZEU 160

Binary Mixture of Deforming Particles — •Yiwei Zhang, Alessandro Manacorda, and Etienne Fodor — DPhyMS, University of Luxembourg, Luxembourg, Luxembourg

Phase separation occurs in miscible liquids where components have distinct properties. In reactors, components undergo stochastic change in their properties which affect the liquid composition. While phase separation and reaction-diffusion have already been studied extensively as separate ingredients, how they combine in non-ideal reactors remains poorly understood. To bridge this gap, we consider repulsive particles with fluctuating size subject to one-body landscape and nonequilibrium synchronisation. The landscape features minima which, regarding size as reaction coordinate, distinguish three states: Particles with finite size, either A- or B-type, and point particles. In this context, synchronisation penalizes A particles in B-rich phases, and vice versa, so that the system eventually accommodates a uniform state. We report the phase diagram depending on the stability of each state and the corresponding particle sizes. Combining hydrodynamic and phenomenological arguments, we recapitulate how metastability regulates the interplay between synchronisation and repulsion. Our results reveal the role of nonequilibrium kinetic factors at play in non-ideal reaction-diffusion systems.

BP 24.11 Thu 12:30 ZEU 160

Self-organization of model catalytic cycles — •Vincent Ouazan-Reboul[1], Jaime Agudo-Canalejo[1], and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, D-37077, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, OX1 3PU, Oxford, UK

We study analytically and numerically a model metabolic cycle composed of an arbitrary number of species of catalytically active parti-

cles. Each species converts a substrate into a product, the latter being used as the substrate by the next species in the cycle. Through a combination of catalytic activity and chemotactic mobility, the catalytic particles develop effective interactions with particles belonging to neighbouring species in the cycle. These interactions, being fully out-of-equilibrium, show some unusual features, in particular being non-reciprocal. We find that such model metabolic cycles are able to self-organize through a macroscopic instability, with a strong dependence on the characteristics of the cycle. For instance, cycles containing an even number of species are able to minimize repulsion between their component particles by aggregating all even-numbered species in one cluster, and all odd-numbered species in another. Such a grouping is not possible if the cycle contains an odd number of species, which can lead to oscillatory steady states in the case of chasing interactions.

BP 24.12 Thu 12:45 ZEU 160

Reentrant condensation transition in a model of driven scalar active matter with diffusivity edge — Berx Jonas[2], •Bose Aritra[1], Mahault Benoit[1], and Golestanian Ramin[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany — [2]Institute for Theoretical Physics, KU Leuven, B-3001 Leuven, Belgium — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

A class of scalar active matter for which the effective diffusivity vanishes beyond a certain density threshold, hereby referred to as diffusivity edge, triggers the formation of a condensate when confined in a harmonic potential. The condensation transition exhibits remarkable similarities with a Bose-Einstein Condensation (BEC). Here we study the effect of a diffusivity edge in a system of scalar active matter confined by a periodic potential and driven by an external force.

We find that this system shows qualitatively distinct stationary regimes depending on the amplitude of the driving force with respect to the potential barrier. For small driving, the diffusivity edge induces a condensation analogous to the BEC-like transition reported for the nondriven case, which is characterised by a density-independent steady state current. Conversely, large external forces lead to a qualitatively different phase diagram where condensation is not possible below a density threshold and the associated transition at moderate densities above the threshold the transition is reentrant due to the existence of a subsequent evaporation transition at low effective temperatures.

BP 25: Cell Mechanics II

Time: Thursday 15:00–17:30 Location: BAR Schö

BP 25.1 Thu 15:00 BAR Schö

Nuclear mechanics probed by optical tweezers-based active microrheology — •Bart Vos[1], Till Münсker[1], Ivan Avilov[2], Peter Lenart[2], and Timo Betz[1] — [1]Third Institute of Physics, University of Göttingen, Göttingen, Germany — [2]Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

Mechanics play a crucial role in a wide range of cellular processes, from differentiation to division and metastatic invasion. Consequently, the mechanical properties of the cytoskeleton, providing shape, motility and mechanical stability to the cell, have been extensively studied. However, remarkably little is known about the mechanical environment within the nucleus of a cell, and fundamental questions remain unanswered, such as the role of nuclear actin or the sudden "freezing" of the cell during cellular division that prevents diffusion or active mixing of the nucleus and the cytoplasm.

To address these questions, we perform optical tweezers-based microrheology in the cellular nucleus. Microrheology has proven to be a suitable tool for intracellular mechanical measurements, as it enables local, non-invasive measurements. However, although the cytoskeleton has been extensively studied this way, the cell nucleus has not been investigated, mainly due to difficulties with inserting appropriate probe particles. By using starfish oocytes that have larger dimensions than most other cell types, we are able to perform microinjection of micrometer-sized particles. We observe viscoelastic behavior of the nucleoplasm that is profoundly different from the cytoskeleton. In addition, we mechanically follow the oocyte during meiotic cell division.

BP 25.2 Thu 15:15 BAR Schö

Mechanosensitive binding of filamins in the actin cytoskeleton of live cells — •Valentin Ruffine and Elisabeth Fischer-Friedrich — DFG Cluster of Excellence Physics of Life, Technische Universität Dresden, Dresden, Germany

Filamins A and B are cross-linkers of the actin cytoskeleton expressed in a wide range of human cell types. In particular, filamins are crucial in actin cytoskeleton interactions with the extracellular matrix and therefore are major molecular players in cartilage and bone development. Filamins form dimers which can bind and cross-link two actin filaments and thus contribute to the mechanical integrity of cytoskeletal structures such as the actin cortex. Myosin-generated contractile tension in the actin cortex is likely translated into a tensile force on the filamin-actin bonds in cross-linking filamins. Filamin binding to actin is transient with unbinding events after a characteristic bond lifetime. This enables large reorganizations of the cytoskeleton at longer timescales. However, tensile force in filamin-actin bonds may affect their unbinding kinetics. Here, we study the binding dynamics of filamins A and B to actin, in the cortex of mitotic HeLa cells. With a set-up combining a confocal and an atomic force microscope, we measure how changes in contractile tension in the actin cortex change filamin binding dynamics. Our results suggest a substantial increase of the lifetime of filamin-actin bonds under increased tensile force. This behavior is termed "catch-binding" and may act as a fast rescue mechanism that prevents rupture of filamin-containing actin cytoskeletal structures upon sudden tension increase.

BP 25.3 Thu 15:30 BAR Schö

T-cell migration: Improving searching efficiency by targeting Microtubules — •Galia Montalvo[1,2,3], Bin Qu[3,4], and Franziska Lautenschläger[1,2,3] — [1]University of Saarland, Department of Experimental Physics — [2]University of Saarland, Center for Biophysics — [3]Biophysics, Center for Integrative Physiology and Molecular Medicine (CIPMM), School of Medicine — [4]Leibniz Institute for New Materials

Cytotoxic T lymphocytes (CTLs) are the key players in the adaptive immune system to eliminate tumor cells. Proper mobility in three-dimensional environments is a prerequisite for CTLs to execute their killing function and the cytoskeleton plays a central role in CTL migration in 3D. In dense matrices, migration and the consequent killing efficiency of CTLs is greatly impaired. Interestingly, we observed that in 3D matrices, CTLs go through narrow quasi-1D channels. Manufactured micro-channels are a recently emerged promising tool with well-defined parameters to investigate cell migration in 1D. In this project, we characterize MTs as a major cytoskeletal component regulating the migration of CTLs in micro-fabricated environments and in dense collagen matrices. To this end, we expose CTLs to MTs disturbing drugs. We studied the mechanics of treated cells and described the role of actin in the observed stiffness increase after MT depolymerization. Our main conclusion is that searching efficiency and killing capacity of CTLs is enhanced after MT depolymerization through stiffness increase.

BP 25.4 Thu 15:45 BAR Schö

Global membrane tension is independent of polyacrylamide substrate stiffness — •Eva Kreysing[1], Jeffrey McHugh[1,2], Sarah Foster[1,3], Kurt Andresen[4], Ryan Greenhalgh[1], Eva Pillai[1,5], Andrea Dimitrcopoulus[1], Ulrich Keyser[1], and Kristian Franze[1,6] — [1]University of Cambridge, UK — [2]Collège de France, Paris — [3]University of Tübingen; Germany — [4]Gettysburg College, USA — [5]EMBL Heidelberg, Germany — [6]University Erlangen/Nürnberg, Germany

Cellular processes such as cell migration or axonal pathfinding have been shown to depend strongly on mechanical properties of the cell*s environment such as stiffness. It has been shown that Piezo1 is one of the mechanosensitive ion channels that contributes to such behaviour. It is hypothesised that Piezo1 is activated by changes in membrane tension. This raises the question whether membrane tension is influenced by stiffness of the cell*s environment. We measured membrane tension as a function of substrate stiffness in different cell types with optical tweezers. To our surprise, we found that global membrane ten-

sion is independent of substrate stiffness in the physiological range. However, we found strong differences between membrane tension on compliant substrates and glass substrates. To explain these observations, this work introduces a toy model for substrate, membrane and cortex interaction.

BP 25.5 Thu 16:00 BAR Schö

Self-stabilization of cell adhesions under load — •Benedikt Sabass — LMU München

Mechanical loading generally weakens adhesive structures and eventually leads to their rupture. However, biological systems can adapt to loads by strengthening adhesions, which is essential for maintaining the integrity of tissue and whole organisms. Inspired by cellular focal adhesions, we discuss generic, molecular mechanisms that enable adhesions to harness applied loads for self-stabilization through adhesion growth. The mechanisms are based on conformation changes of adhesion molecules that are dynamically exchanged with a reservoir. Tangential loading drives the occupation of some states out of equilibrium, which, for thermodynamic reasons, leads to association of further molecules with the cluster. The self-stabilization principle can be realized in many ways in complex adhesion-state networks and we show how it naturally occurs in cellular adhesions involving the adaptor proteins talin and vinculin.

Braeutigam, A., Simsek, A.N., Gompper, G., and Sabass, B., Nature Communications 13(1):1-9, 2022

15 min. break

BP 25.6 Thu 16:30 BAR Schö

Unraveling the light activation of flagellar adhesiveness in *Chlamydomonas* — •Rodrigo Catalan[1,2], Antoine Girot[1,2], Alexandros Fragkopoulos[1,2], Simon Kelterborn[3], Darius Rauch[3], Olga Baidukova[3], Peter Hegemann[3], and Oliver Bäumchen[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [2]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [3]Humboldt University Berlin, Institute of Biology, 10115 Berlin, Germany

Photoreceptors are essential constituents of photoactive microbes and control several biological processes, such as circadian life cycle, sexual reproduction and phototaxis. *Chlamydomonas reinhardtii*, a unicellular model organism to study light-activated microbial functionalities, exhibits light-switchable flagellar adhesion to surfaces upon blue-light exposure [Kreis *et al.*, Nature Physics 2018]. Using single-cell micropipette force spectroscopy, we compare the adhesion forces of wild-type (WT) cells and several blue-light photoreceptor-deletion mutants. We find that the wavelength response of flagellar adhesion forces in WT cells resembles the absorption spectrum of plant cryptochrome (pCRY) and animal cryptochrome (aCRY) photoreceptors. We further assess the involvement of pCRY and aCRY photoreceptors in the light-switchable adhesion of *C. reinhardtii* by means of adsorption experiments [Catalan *et al.*, arXiv:2208.01338] at the population level using photoreceptor-deletion mutants lacking either one or both CRYs.

BP 25.7 Thu 16:45 BAR Schö

Chromatin and Nucleocytoplasmic Transport Control the Nuclear Biophysical Properties during Assembly in Egg Extracts — •Omar Muñoz[1,2], Abin Biswas[1,4], Kyoohyun Kim[1,3], Simone Reber[4], Jochen Guck[1,3], and Vasily Zaburdaev[1,2] — [1]Max-Planck-Zentrum für Physik und Medizin — [2]Department of Biology, Friedrich-Alexander-Universität Erlangen-Nürnberg — [3]Max Planck Institute for the Science of Light — [4]IRI Life Sciences, Humboldt-Universität zu Berlin

Biophysical properties of the cell nucleus are important for various cellular processes from migration to stress responses, but largely are still not well understood. One fundamental example is the mass density: we observed that the nuclear mass density consistently displays a lower value than its cytoplasmic counterpart for a wide range of species, which is surprising given that it contains the highly compacted genetic material. To understand the mechanisms behind this, we measured volume and mass density of growing nuclei reconstituted in Xenopus egg extracts. Our results identified nucleocytoplasmic transport and chromatin as the main determinants for the dry mass and volume of then nucleus, and suggest a coupling of chromatin with nucleocytoplasmic transport. We propose a theoretical model informed by experiments, which incorporates active transport of proteins and balance of colloid osmotic pressure and an entropic polymer pressure exerted by chromatin. With only a few adjustable parameters, our model can fully describe the nuclear volume and mass dynamics as observed in the experiments.

BP 25.8 Thu 17:00 BAR Schö

Dyneins, unite! How a weak motor protein can drive efficient transport of large cargoes — •Simon Wieland[1,2], Christina Steininger[1], David E. Gitschier[1], Marius M. Kaiser[1], Wolfgang Gross[1], Abdullah R. Chaudhary[3], Jana Ritschar[4], Christian Laforsch[2], Adam G. Hendricks[3], and Holger Kress[1] — [1]Biological Physics, University of Bayreuth, Germany — [2]Animal Ecology I, University of Bayreuth, Germany — [3]Department of Bioengineering, McGill University, Montreal, Canada — [4]Laboratory of Molecular Parasitology, University of Bayreuth, Germany

To promote robust transport of organelles, dyneins need to work together to overcome intracellular drag forces and opposing forces of kinesins. However, current models of dynein cooperativity cannot explain how dyneins produce very high forces to power transport of large organelles with diameters of several microns. Here, we show that many dynein teams interact with multiple microtubules to drive efficient transport of large organelles. We measured retrograde transport forces of phagosomes with diameters of 1-5 μm. These forces were adapted to the cytoplasmic viscosity, enabling equally fast transport of all phagosomes. Furthermore, we labeled and quantified dyneins on isolated phagosomes. By modeling the distribution of microtubules around the phagosomes we linked the observed transport forces to the corresponding dynein numbers. We show that both dynein's cooperativity and size-dependent interactions of organelles with microtubules contribute to the production of high collective transport forces.

BP 25.9 Thu 17:15 BAR Schö

The formation of microtentacles — •Lucina Kainka[1], Reza Shaebani[2,3], Kathi Kaiser[1], Ludger Santen[2,3], and Franziska Lautenschläger[1,3] — [1]Department of Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Department of Theoretical Physics, Saarland University, Saarbrücken, Germany — [3]Center for Biophysics, Saarland University, Saarbrücken, Germany

It is widely assumed that cellular stiffness decreases during cancer progression, and this is mainly attributed to changes in their actin cortex properties. It has recently been proposed that a weakened actin cortex enables the formation of so called microtentacles. Microtentacles are microtubule-based membrane protrusions that are formed by circulating tumor cells. It is assumed that microtentacles promote reattachment of circulating tumor cells to the tissue and the escape from the blood stream.In this study, we aim to understand how the actin cortex structure changes during cancer progression to enable microtentacle formation. We further ask how microtubules generate forces to protrude the cell membrane.In our experiments, we use noncancer RPE-1 cells as a model system. By treating these cells with actin affecting compounds while they are in suspension, they form microtentacles. We further can control the number and length of microtentacles by varying the concentration of compounds applied. We analyze the actin cortex and microtubule network in these cells with fluorescence and scanning electron microscopy. We further study the microtubule dynamics inside microtentacles by fluorescence recovery after photobleaching (FRAP).

BP 26: Focus Session mRNA Physics

Time: Thursday 15:00–17:30 Location: TOE 317

Invited Talk BP 26.1 Thu 15:00 TOE 317

Decoding Molecular Plasticity in the Dark Proteome of the Nuclear Transport Machinery — •Edward Lemke — JGU & IMB Mainz, GE

The mechanisms by which intrinsically disordered proteins (IDPs) engage in rapid and highly selective binding is a subject of considerable interest and represents a central paradigm to nuclear pore complex (NPC) function. Nuclear transport receptors (NTRs) can move small proteins and mRNA through the central channel of the NPC which is filled with hundreds of phenylalanine-glycine-rich nucleoporins (FG-Nups) reaching millimolar concentrations with elusive conformational plasticity. We have now developed a semi-synthetic strategy to equip the living cell with up to three genetic codes and label FG-Nups inside functional NPCs site-specifically with small FRET probes. This allowed us to develop an experimental approach and use fluorescent lifetime imaging microscopy (FLIM) to directly decipher the plasticity of FG-Nups. Our study enabled a conformational look on the densely packed IDPs in the sub-resolution (roughly (50 nm)^3 small cavity) cavity of the NPC. We extracted the scaling exponent, which directly describes the conformations of FG-Nups at their functional status as well as the solvent quality in the cellular and even inner NPC environment. Pairing our data with coarse grained simulations enabled us to complement the missing half of protein mass that due to its dynamics are not present in even the most recent electron tomograms of the NPC.

BP 26.2 Thu 15:30 TOE 317

Decomposition of ensemble fluorescence signals from translation experiments and simulations — •Nadin Haase, Simon Christ, and Sophia Rudorf — Institute of Cell Biology and Biophysics, Leibniz University Hannover, Germany

Proteins are major components of cells and perform all kinds of tasks essential for survival. Those parts of the DNA that contain blueprints for the synthesis of proteins are transcribed to messenger RNA (mRNA). Complex biomolecular machines called ribosomes translate the mRNA by assembling the corresponding building blocks of proteins, the amino acids. This process can be studied by in-vitro ensemble experiments through monitoring time-dependent output signals such as fluorescence time traces, where the ensemble signal is a superposition of the individual signals from all molecules in the reaction. However, translation is a stochastic process and thus even for initially synchronized reactions the ensemble signal may not reflect the features in the individual signals, especially on longer time scales. Here we present an approach to decompose the ensemble signal to reveal hidden information about the individual steps of the translation process. We explore the limits of this method and study the conditions under which a meaningful solution can be gathered.

BP 26.3 Thu 15:45 TOE 317

Creating an evolution machine with 2-3-cyclic RNA — •Dieter Braun — Systems Biophysics, Ludwig Maximilian University Munich

For life to start, a simple physical non-equlibrium mechanism combined with a most robust chemistry of a few molecules had to reach the regime of Darwinian molecular evolution. We found RNA oligomerization and templated ligation from very mildly activated RNA with 2-3-cyclic phosphates [1], with wet-dry cycling at heated air-water interfaces [2]. The oligomerization operated at elevated pH 9-10 without added salts at temperatures between 4-40°C and created oligomers of all four bases with 15 percent yield. It operated in a water-poor 'dry' state. Replication was possible with templated ligation and showed with only 1mM MgCl2 a strongly base-selective templated ligation with 25 percent yield. If catalytic conditions to recycle the hydrolytically opened 2-3-cyclic phosphate from linear 2 prime or 3 prime endings wcould be found, the reaction would operate indefinitely without feeding in a thermal gradient setting. We will show preliminary experiments for local feeding, vesiculation and protein expression in the same setting. The experiments suggest a most simple scenario for the emergence of life from only two nucleotide molecules, implemented in an early Earth volcanic setting under a CO2 atmosphere. It showcases how physics and chemistry could have acted together in a geologically abundant microfluidic setting to create Darwinian evolution.

[1] ChemSystemsChem doi.org/10.1002/syst.202200026 (2022)
[2] Nature Physics doi.org/10.1038/s41567-022-01516-z (2022)

BP 26.4 Thu 16:00 TOE 317

RNA G-quadruplex folding is a multi-pathway process with a variety of short-lived intermediate states — •Marijana Ugrina[1], Ines Burkhart[2], Diana Müller[2], Harald Schwalbe[2], and Nadine Schwierz[1] — [1]University of Augsburg, Augsburg, Germany — [2]Goethe University, Frankfurt am Main, Germany

The folding kinetics of regulatory RNAs is crucial for their function. Here, we provide molecular insights into the folding pathways of a G-quadruplex from telomeric repeat-containing RNA by combining all-atom molecular dynamics and coarse-grained simulations with circular dichroism experiments. The ion atmosphere surrounding the highly charged quadruplex plays a crucial role in folding. To correctly capture the electric double-layer in implicit solvent coarse-grained simulations, we develop a matching procedure based on all-atom simulations in explicit water. This procedure allows us to provide quantitative agreement between the experiments and simulations as judged by the number of native contacts at different salt concentrations and temperatures. Folding of the quadruplex is on the timescale of minutes and the coarse-grained simulations using the three-interactions site model are therefore ideal to resolve the folding pathways and intermediate states. The results reveal that the folding is sequential with each pathway passing through two transient, on-pathway intermediates: A hairpin and a triplex or double hairpin state. Since these intermediates are degenerate with at two to four alternative conformations per state, quadruplex folding is a multi-pathway process with high conformational entropy.

15 min. break

BP 26.5 Thu 16:30 TOE 317

Codon position-specific engineering of translation kinetics — Judith Müller[1], Gerlinde Schwake[1], Anita Reiser[1], Daniel Woschée[1], Zahra Alirezaeizanjani[3], Joachim Rädler[1], and •Sophia Rudorf[2] — [1]Faculty of Physics, Ludwig Maximilian University of Munich — [2]Faculty of Natural Sciences, Leibniz University Hannover — [3]independent researcher

Recently, we introduced Live Imaging on Single Cell Arrays (LISCA), which combines time-lapse microscopy of single cells on microstructured surfaces with automated image analysis. LISCA enables us to observe and analyze the time-evolution of protein expression in hundreds of individual cells in parallel. Here, we combine LISCA with our software OCTOPOS, which simulates ribosome movement on the ORF and is used to generate reporter genes with varying ribosome speeds and densities. We predict and monitor the translation kinetics of synonymous variants of eGFP to determine mRNA functional lifetimes and translation rates with high accuracy in single lung tissue cells. Our approach allows us to study how provoked ribosome jams on specific positions within the ORF influence mRNA stability, thus linking ribosome dynamics and mRNA biophysics.

BP 26.6 Thu 16:45 TOE 317

The pH dependent phase transition in lipid nanoparticle cores leads to changes of protein expression in single cells — •Julian Philipp and Joachim Rädler — LMU, Munich, Germany

Lipid nanoparticles developed into the most powerful delivery platform for mRNA-based vaccination and therapies. In general, LNPs are particles exhibiting PEG-lipid and DSPC at the surface and ionizable lipid, cholesterol and mRNA in the core. However, the pH dependent changes induced by ionizable lipids in the context of endosomal release are little understood. In particular the ionizable lipids MC3, KC2 and DLin are known to exhibit remarkably different efficacy despite similar pK values. Here, we study the structural response of ionizable lipids with cholesterol as a function of pH using synchrotron X-ray scattering. All three core phases exhibit a sequence of ordered mesophases in the range of pH 7 to 4, beginning with an isotropic swollen phase above their pK value. Lowering the pH reveals transitions to inverse micellar $P6_3/mmc$ / $Fd3m$, inverse hexagonal H_{II} and bicontinous cubic $Pn3m$ phases. If polyA, as mRNA surrogate, is added to the core phases, coexistence of pure lipid phases and condensed nucleic acid

lipid H_{II}^c phase occurs. We show that the observed core structures are consistent with the SAXS scattering of mRNA containing core phases and full LNP. The difference in structural features of DLin versus MC3 and KC2 phases is also consistent with the delayed onset and reduced level of GFP expression observed in single cell time courses after transfection with DLin LNPs compared to MC3/KC2. We conclude that pH dependent core phase transitions trigger endosomal release.

BP 26.7 Thu 17:00 TOE 317

pH-dependent behavior of ionizable cationic lipids in mRNA-carrying lipoplexes investigated by molecular dynamics simulations — •Giovanni Settanni[1,2], Wolfgang Brill[3], Heinirich Haas[3], and Friederike Schmid[1] — [1]Department of Physics, Johannes Gutenberg University Mainz, Germany — [2]Faculty of Physics and Astronomy, Ruhr University Bochum, Germany — [3]BioNTech SE, Mainz, Germany

Lipid-based nanoparticles and lipoplexes are successful nanocarriers for mRNA-based therapies. The molecular structure of these assemblies is still not fully understood. Lipoplexes including the ionizable lipid 2-dioleyloxy-N,N-dimethyl-3-aminopropane (DODMA), under specific conditions, have a pH-dependent lamellar structure, where lipid bilayers are separated by mRNA-rich layers. Here, the structure and dynamics of these lipoplexes are investigated at varying pH and mRNA-concentration using multiscale molecular dynamics simulations[1]. It is observed that the interaction between DODMA and RNA is slightly attractive only at low pH levels. This results into a pH-dependent relocation of the RNA inside the multilayers, from bilayer's surface at low pH to a more uniform distribution inside the hydrophilic slabs at high pH. Also, at high pH, DODMA lipids shift toward the hydrophobic part of the bilayer, thus increasing their leaflet-flipping rate, a phenomenon which may ultimately affect the fusion process of the lipoplex with the endosomal membrane.

[1] Settanni, G., Brill, W., Haas, H. and Schmid, F. (2022), Macromol. Rapid Commun. 43:2100683. https://doi.org/10.1002/marc.202100683

BP 26.8 Thu 17:15 TOE 317

Charge and structural properties of transfection lipid layers adsorbing mRNA — •Miriam Grava[1], Ibrahim Mohd[2,3], Julio Pusterla[1], Julian Philipp[4], Joachim Rädler[4], Olaf Soltwedel[1], Nadine Schwierz[2,3], Heinrich Haas[5], and Emanuel Schneck[1] — [1]Technische Universität Darmstadt, Germany — [2]University of Augsburg, Germany — [3]Max-Planck-Institute of Biophysics, Frankfurt am Main, Germany — [4]Ludwig-Maximilians-Universität München, Germany — [5]BioNTech Corporation, Mainz, Germany

Some of the most effective COVID-19 vaccines are based on cationic lipid-based delivery systems for messenger RNA (mRNA), a promising technology for a broader use in biomedical applications. Its efficiency depends on pH variations and ionic conditions of the bulk phase. We combine x-ray scattering and x-ray fluorescence on monolayers of positively chargeable transfection lipid mixtures with atomistic molecular dynamics (MD) simulations in order to determine their pH-dependent structural properties and the protonation degree. While the experiments yield electron density profiles and surface charge densities, the MD simulations yield the area per molecule, the conformation of different lipid species, and the counter-ion distributions. The analysis of experimental and simulation data provides detailed information on the transfection lipid layer characteristics. We applied the same experimental techniques to transfection lipid layers before and after mRNA adsorption, which yields insights into the structure of the adsorbed layers and the interfacial electrostatic balance.

BP 27: Computational Biophysics II

Time: Thursday 15:00–17:30 Location: BAR 0106

BP 27.1 Thu 15:00 BAR 0106

Spectral signatures of excess-proton waiting and transfer-path dynamics — •Florian Brünig[1], Manuel Rammler[1], Ellen Adams[2], Martina Havenith[2], and Roland Netz[1] — [1]Freie Universität Berlin, Department of Physics, 14195 Berlin, Germany — [2]Ruhr-Universität Bochum, Department of Physical Chemistry II, 44780 Bochum, Germany

Signatures of solvated excess protons in infrared difference absorption spectra, such as the continuum band between the water bend and stretch bands, have been experimentally known for a long time and have recently been used to analyze protonation dynamics in photoactive proteins. However, the theoretical basis for linking spectral signatures with the microscopic proton-transfer mechanism so far relied on normal-mode analysis.

We analyze the excess-proton dynamics in ab initio molecular-dynamics simulations of aqueous hydrochloric acid solutions by trajectory-decomposition techniques. The continuum band is shown to be due to normal-mode oscillations of temporary H_3O^+ complexes. The actual proton transfer between two water molecules, which for large water separations involves crossing of a barrier and thus is not a normal mode, is characterized by two time scales: Firstly, the waiting time for transfer to occur, which leads to a broad weak shoulder around 100 cm^{-1}, consistent with our experimental THz spectra. Secondly, the mean duration of a transfer event, which produces a rather well-defined spectral contribution around 1200 cm^{-1} and agrees in location and width with previous experimental spectra.

BP 27.2 Thu 15:15 BAR 0106

Lipid-based nanomaterials for RNA delivery investigated using molecular dynamics simulations — •David Noel Zimmer[1] and Giovanni Settanni[1,2] — [1]Physics Department University of Mainz — [2]Faculty of Physics and Astronomy Ruhr University Bochum

Lipid-based nanoparticles (LNP) are one of the most effective carriers in mRNA therapeutics. They are made of a mixture of ionizable, helper, and pegylated lipids encapsulating mRNA. While peg tends to remain on the surface of the nanoparticle, the structure of the core has not yet been well characterized. Experimental data point to a relative lack of order. The lipid composition of the formulation plays a key role in determining the effectiveness of the nano carrier. Small changes in the chemical structure of ionizable and helper lipids dramatically affect the efficiency of mRNA transfection. LNPs based on DLinDMA and DLinDAP, two ionizable lipids, showed significantly different transfection efficiencies, notwithstanding the very small difference in structure. Here, using a multiscale modeling approach, the behavior of lipid formulations based on these two lipids, cholesterol and DSPC or DOPE is examined aiming to provide an understanding of the interactions of lipids and mRNA. The simulations show that, despite DLinDAP binding affinity for mRNA is larger than DLinDMA, the overall interaction of the whole lipid formulation containing DLinDAP with mRNA is weaker, resulting in a larger average distance of the mRNA from the lipid bilayer. This shows that chemical optimization based only on mRNA-ionizable lipid interactions may not be sufficient for the development of more effective lipid formulations for RNA delivery.

BP 27.3 Thu 15:30 BAR 0106

Toehold-Mediated Strand Displacement in Random Sequence Pools — •Thomas Mayer, Lukas Oesinghaus, and Friedrich Simmel — School of Natural Sciences, Department of Bioscience, TU Munich, D-85748 Garching, Germany

Toehold-mediated strand displacement (TMSD) has been used extensively for molecular sensing and computing in DNA-based molecular circuits. As these circuits grow in complexity, sequence similarity between components can lead to cross-talk causing leak, altered kinetics, or even circuit failure. For small circuits, such unwanted interactions can be designed against. In environments containing a huge number of sequences, this becomes infeasible. Therefore, a general understanding of the impact of sequence backgrounds on TMSD reactions is of great interest. Here, we investigate the impact of random DNA sequences on TMSD circuits. We begin by studying individual interfering strands and use the obtained data to build machine learning models that estimate kinetics. We then investigate the influence of pools of random strands and find that the kinetics are determined by only a small subpopulation of strongly interacting strands. Consequently, their behavior can be mimicked by a small collection of such strands. Finally, we compare two established and a novel technique that speed up TMSD reactions in random sequence pools: a threeletter alphabet, protection of toeholds by intramolecular secondary structure, or by an additional

blocking strand. We expect that our insights will be useful for the construction of TMSD circuits that are robust to molecular noise.

BP 27.4 Thu 15:45 BAR 0106

comparison of molecular dynamics simulations and neutron reflectivity experiments reveals strengths and weaknesses of current force fields for ionizable Dlin-MC3-DMA lipids — •Ibrahim Mohd[1,3], Jennifer Gilbert[2], Marcel Heinz[3], Tommy Nylander[2], and Nadine Schwierz[1,3] — [1]University of Augsburg, 86159 Augsburg, Germany — [2]Lund University, SE-22100 Lund, Sweden — [3]Max-Planck-Institute of Biophysics, 60438 Frankfurt am Main, Germany

Dlin-MC3-DMA (MC3) is one the most promising ionisable lipid for designing lipid nanoparticles (LNPs), which are used as drug delivery agents. Here, we provide force field parameters for cationic and neutral MC3 compatible with the AMBER Lipid17 force field. Subsequently, we carefully assess the accuracy of the current and existing MC3 force fields by providing a direct comparison to neutron reflectivity experiments of mixed lipid bilayers consisting of MC3 and DOPC at different pH. At low pH (cationic MC3) and at high pH (neutral MC3) the newly developed MC3 parameters in combination with AMBER Lipid17 for DOPC give excellent agreement with the experiments compared to existing MC3 models. With the currently parametrized MC3 parameters we are able to simulate MC3 containing LNPs in atomistic details and gain insights into the effect of pH and RNA cargo on the LNP structure. Combining molecular dynamics simulations, neutron reflectivity experiments and other scattering techniques is therefore a valuable step to drive the advancement of accurate atomistic force fields and to unravel the detailed structure of LNPs.

BP 27.5 Thu 16:00 BAR 0106

Simulation-based Parameter Inference for Large Scale Tumor Simulations — •Julian Herold[1], Eric Behle[2], and Alexander Schug[2] — [1]Karlsruhe Institute of Technology, Karlsruhe, Deutschland — [2]Jülich Supercomputing Center, Jülich, Deutschland

While clinical imaging of tissues focuses on macroscopic tumors, many experiments investigate only small clusters of cells. We aim on providing a scale-bridging link by performing large scale tissue simulations. We employ highly parallelized code in an HPC setting to simulate mm-sized virtual tissues such as embryogenetic zebrafish tissue or breast-cancer tumors with more than a million μm-resolved individual cells. We deploy Cells in Silico (CiS), which combines a cellular potts model with an agent based layer and is thus capable of accurately representing many physical and biological properties, such as individual cell shapes, cell division, cell motility, interactions with the extra-cellular matrix etc.

Using a model with such a strong representational capacity poses the task of adjusting a large number of parameters to reproduce experimental findings. Prior work has attempted to characterize the similarity between experimental and simulated data by extracting different features and using statistical tests to establish a distance measure. This work highlights how this difficult task can be circumvented by training neural networks to distinguish between experimental and simulated data while simultaneously optimizing the model parameters to maximize the error rate of the network.

15 min. break

BP 27.6 Thu 16:30 BAR 0106

Effects of chromatin fibers characteristics on cohesin mediated loop architecture — •Aymen Attou, TIlo Zülske, and Gero Wedemann — University of Applied Sciences Stralsund, System Engineering and Information Management, 18435 Stralsund, Germany

The spatial organization of DNA in eucaryotes starts at nucleosome chains forming chromatin loops that can cluster together establishing fundamental units called topologically associating domains (TADs). TADs are an important factor for gene regulation by facilitation or repressing long range contacts in the genome. Those loops are formed and held together by a ring-shaped protein complex called cohesin together with the effect of CTCF. A loop has a residence time of several minutes. To clarify the spatial structure of a loop, we established a coarse-grained computer model of chromatin with a resolution of single nucleosomes integrating potentials describing CTCF and cohesin. We performed Metropolis Monte Carlo simulations combined with replica exchange procedure with regular spaced nucleosomes and experimentally determined nucleosome positions in presence of cohesin-CTCF as well as depleted systems as control for different loop sizes. We studied differences in the spatial structure and of contacts probabilities of different domains, what allowed us to understand the role of cohesin and CTCF, and their impact on the 3D structure of chromatin. This study also allowed clarifying how nucleosome positions can impact the conformations of the chromatin loops during the residence time of the loop anchor, with presumed consequences for transcriptional activity.

BP 27.7 Thu 16:45 BAR 0106

Theoretical investigations on enzyme-plasma interactions in the context of plasma-driven biocatalysis — •Hanna-Friederike Poggemann, Björn Kirchhoff, Timo Jacob, and Christoph Jung — Ulm University, Institute of Electrochemistry, D-89069 Ulm

Biocatalysis is an emerging field that has several advantages over classical catalysis. The use of enzymes as catalysts is not only more environmentally friendly, but also has potential to be more efficient than the conventional approach in industrial applications. Plasma-assisted biocatalysis is a specific subsection of this field, where a plasma source is used to provide a constant supply of the enzyme co-substrate H_2O_2 that drives the catalytic reaction. However, the use of plasma presents some challenges. The plasma species can alter the structure of the enzyme leading to changes in the catalytic reaction pathway or even deactivation of the enzyme. In a theoretical multiscale approach, we address the questions of how the plasma interacts with the enzyme and how this alters the catalytic reaction. To this end, we use reactive molecular dynamics simulations to investigate possible structural changes of the enzyme by plasma species. We also perform QM/MM hybrid simulations to further investigate the reaction pathway of the enzyme AaeUPO.

BP 27.8 Thu 17:00 BAR 0106

Diffusive properties in simulations of polydisperse sphere mixtures mimicking the inside of a cell — •Frank Hirschmann[1], Hender Lopez[2], Felix Roosen-Runge[3], and Martin Oettel[1] — [1]Institute for Applied Physics, University of Tübingen, Germany — [2]School of Physics and Optometric & Clinical Sciences, Technological University Dublin, Ireland — [3]Department of Biomedical Sciences and Biofilms-Research Center for Biointerfaces (BRCB), Malmö University, Sweden

The interiors of living cells contain a multitude of different-sized biomacromolecules at relatively high packing fractions. Diffusivity and transport properties in such crowded environments are highly influenced by hydrodynamic interactions. Thus, the time needed for proteins to come into contact with each other within the cell is determined by a complex interplay of polydispersity, size-distribution and crowding. In order to analyze such systems theoretically, we employ Brownian Dynamics (BD) simulations of polydisperse mixtures of hard spheres. Using results of Stokesian dynamics we approximate hydrodynamic interactions in our BD simulations by a simple multiplicative ansatz (equivalent to a hydrodynamic "renormalization" of the Brownian short-time diffusivity), which allows us to access the long-time limit of our system. We investigate resulting diffusion constants and survival probabilities, exhibiting non-trivial behavior.

BP 27.9 Thu 17:15 BAR 0106

Unwrapping trajectories of constant-pressure molecular dynamics simulations — •Jakob Tómas Bullerjahn[1], Sören von Bülow[2], Jérôme Hénin[3], and Gerhard Hummer[1,4] — [1]Department of Theoretical Biophysics, Max Planck Institute of Biophysics, Frankfurt am Main, Germany — [2]Linderstrøm-Lang Centre for Protein Science, Department of Biology, University of Copenhagen, Copenhagen, Denmark — [3]Laboratoire de Biochimie Théorique, Institut de Biologie Physico-Chimique, CNRS, Paris, France — [4]Institute of Biophysics, Goethe University Frankfurt, Frankfurt am Main, Germany

In molecular dynamics simulations at constant pressure, the size and shape of the periodic simulation box fluctuate with time. Special care is thus required when a particle trajectory is unwrapped from a projection into the central box under periodic boundary conditions into a trajectory in full three-dimensional space, e.g., for the calculation of diffusion coefficients. Here, we review and compare different schemes proposed for trajectory unwrapping, and specify the respective rewrapping scheme to put an unwrapped trajectory back into the central box. On this basis, we then identify a scheme in which the wrapped and unwrapped trajectory are mutually consistent and in which the statistical

properties of the trajectory are preserved. We conclude with advice on best practice for the consistent unwrapping of constant-pressure simulation trajectories.

BP 28: Poster Session II

Time: Thursday 18:00–20:00 Location: P2/EG

BP 28.1 Thu 18:00 P2/EG

X-Ray Phase-Contrast Tomography Imaging of Single Cells Using an Optical Stretcher — •Jan-Philipp Burchert[1], Roland Stange[2], Madleen Busse[3], Tim Salditt[1], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen — [2]RS Zelltechnik GmbH, Schöllnach — [3]Department of Physics and Munich School of Biomedical Engineering, Technical University of Munich

X-rays penetrate deep into matter and allow us to image structures with high spatial resolution, which makes them attractive for investigating individual biological cells. Here, we combine x-ray phase-contrast tomography with an x-ray compatible optical stretcher to image single cells in solution, thus in their physiological environment, and avoid the need for freezing, drying or embedding of the samples. The cells are trapped in a contact-free manner in a fixed position by the optical stretcher and are probed by the x-ray beam. The microfluidic flow sets the cells in slow rotational motion, which enables tomographic imaging. We apply this combination of techniques to unfixed and fixed NIH3T3 fibroblasts, which are partially stained with an x-ray contrast agent. The experimental data show that we can acquire images of these cells with our setup. Moreover, the comparison of the different preparations and two beam energies will improve the image quality in future experiments.

BP 28.2 Thu 18:00 P2/EG

Scanning small angle x-ray scattering of hydrated, keratin-rich cells in flow environment — •Boram Yu[1], Sophie-Charlotte August[1], Peter Luley[1], Manfred Burgerhammer[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen, Germany — [2]European Synchrotron Radiation Facility (ESRF), Grenoble, France

Intermediate filaments (IFs), one of the three main components of the cytoskeleton, form a network that contributes to cell mechanics. Thus, collecting structural information about IF networks in their physiological setting, i.e., in whole living cells, is crucial. We study mammalian cells expressing cytokeratin, which forms bundle structures. To obtain this information, we use scanning small angle x-ray scattering (SAXS), as it provides both real space overview images with moderate resolution and reciprocal space information with a high resolution. X-ray imaging of cells in aqueous state is challenging as their electron density contrast is low, and pronounced radiation damage and radiation-induced gas formation occurs. For this reason, we used a dedicated flow sample chamber that minimizes the thickness of liquid layer in the beam path and serves to exchange liquid continuously during scanning. Despite weak contrast and short exposure times, we are able to retrieve the local main orientation of subcellular structures, thus demonstrating how scanning SAXS offers valuable information from fixed-hydrated cells in liquid flow.

BP 28.3 Thu 18:00 P2/EG

Comparative investigation of differently prepared porcine retinal pigment ephitelium (RPE) cells using mid-IR photo-induced force microscopy (PiF-IR) — •Jesvin Joseph[1,2], Robin Schneider[1], Rowena Simon[3], and Daniela Täuber[1,2,4] — [1]Heintzmann Lab, Leibniz Institute of Photonic Technology, Jena — [2]Institute of Physical Chemistry & Abbe Center of Photonics, Friedrich-Schiller-University Jena — [3]Department of Ophthalmology, University Hospital Jena — [4]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

Age-related loss of sight caused by macular degeneration (AMD) is monitored in clinical health care using fundus autofluorescence, which investigates variations in the autofluorescence signal stemming from the retinal pigment epithelium (RPE)[1]. Nanolocal chemical characterization of RPE cells and pigment granules could deepen the understanding of involved cellular processes. Nano-infrared imaging methods can provide chemical information at a lateral resolution below 10 nm[2]. We used PiF-IR to investigate externally grown porcine RPE cells, which were dried in varied conditions. First results show spectral variations obtained from cells dried at room temperature and at 37°C. We compare these spectra to PiF-IR and conventional FTIR spectra obtained from plain retinal pigment chemicals. Funding by Profil Line Light, project pintXsum, FSU Jena, is acknowledged. [1] Schultz, R., Schwanengel, L., Klemm, M., Meller, D. & Hammer, M. Acta Ophthalmologica (2021). [2] Luo, X. Xue, Y.; Wu, J.; Cai, W.; Täuber, et al. Applied Physics Letters DOI: 10.1063/5.0128850.

BP 28.4 Thu 18:00 P2/EG

Redirecting the early embryogenesis of *Caenorhabditis elegans* by altering mechanical cues — •Vincent Borne and Matthias Weiss — Experimental Physics I, University of Bayreuth, Universitätsstr. 30, D-95447 Bayreuth, Germany

During early development, somatic and germline precursor cells of the model organism *Caenorhabditis elegans* undergo an apparently predetermined and robust division scheme, suggesting early embryogenesis to run on autopilot. While the role of biochemical signaling in embryogenesis has long been recognized, the influence of mechanical forces for proper cell arrangement has been revealed only recently. Aiming at challenging the robustness of the organismal development mechanically, we have flattened the embryo to induce altered positioning and division timing of cells. Indeed, upon a controlled squeezing between two coverslips, the outer boundary of the embryo remained intact but cytokinesis was seen to be compromised, i.e. normal development came to a full stop. Surprisingly, nuclei still underwent division, resulting in multinucleated cells or even a syncytium-like state with up to 60 nuclei. In this state, we have monitored the growth of nuclei and their division timing. Despite the total failure of cell division, both observables are in line with experimental data and theoretical descriptions obtained from unperturbed embryos. Our results highlight how some key features for correct embryonic development prevail even under mechanically stressful conditions.

BP 28.5 Thu 18:00 P2/EG

Microfluidics-based analysis of the mobility and migration pattern of *Trypanosoma brucei* — •Hannes Wunderlich[1], Lucas Brehm[2], Jana Ritschar[2], Sebastian Krauss[1], Klaus Ersfeld[2], and Matthias Weiss[1] — [1]Experimental Physics I, University of Bayreuth, Germany — [2]Molecular Parasitology, University of Bayreuth, Germany

Trypanosoma brucei is a unicellular parasite that causes the African sleeping sickness after entering the human bloodstream via the bite of an infected tsetse fly. Active spiral movement of trypanosomes, mediated by the beating of a microtubule-driven cell-body attached flagellum, is crucial to evade the hosts immune response, i.e. swimming is a matter of survival for trypanosomes. Beyond the flagellum, microtubules also form a highly ordered, subpellicular array beneath the cell membrane, hence determining the effective elasticity of the parasite and its propulsion via the flagellum. Using soft lithography to produce well-defined two-dimensional chambers and using a temperature controlled environment, we have optimized cell tracking, shape determination, and subsequent analyses. As a result, we find that wild-type and mutant strains with altered post-translational modifications of microtubules not only feature different phenotypes but also show distinct mobility patterns, e.g. a strain-dependent swimming velocitiy and intermittency of swimming (run-and-tumble phases).

BP 28.6 Thu 18:00 P2/EG

2D polarization fluorescence imaging (2DPOLIM) - Evaluation of depolarization artifacts in fixed four channel detection — •Yunhao Mei[1,2], Asad Hafeez[1,2], Yutong Wang[1,2], Mohammad Soltaninezhad[1,2], Rainer Heintzmann[1,2], and Daniela Täuber[1,2] — [1]Heintzmann Lab, Leibniz Institute of Photonic Technology, Jena — [2]Institute of Physical Chemistry & Abbe Center of Photonics, Friedrich-Schiller-University Jena, Germany

Fluorescence polarization and anisotropy measurements are widely used in Diagnostics and Imaging in the Life Sciences. Most common is the use of linearly polarized excitation together with two-channel

detection of linear polarization parallel and perpendicular to the polarization in excitation. However, when applied to anisotropic samples, the result may depend on the lab frame in respect to structural alignments within the sample, which can be preventend by collecting the sample fluorescence in more polarization angles[1]. We designed a four-channel detection for evaluating Förster Resonance Energy Transfer between similar fluorescence labels, the so-called homo-FRET or em-FRET. The quantitative discrimination of FRET via tiny changes in polarization resolved fluorescence intensities requires highly sensitive cameras and well-designed and calibrated detection channels. Wire grids provide high-quality polarization properties when used in normal incidence in transmission but may introduce depolarization when implemented tilted in respect to the optical axis. We studied several possible arrangements and compared the introduced depolarizations. [1] R. Camacho et al. Adv. Mater. 2019, 1805671.

BP 28.7 Thu 18:00 P2/EG

Monitoring actomyosin flows in early Caenorhabditis elegans embryos by lightsheet microscopy — •Ivana Jeremic and Matthias Weiss — University of Bayreuth, Bayreuth, Germany

Symmetry breaking, i.e. the formation of body axes, is crucial for embryonic development as it guides the formation of highly organized tissues and consequently assures proper maturation of the organism. A convenient model system for studying such events is Caenorhabditis elegans since all body axes are fully defined already in the 8-cell stage of the embryo. Confocal fluorescence imaging on C. elegans has revealed that chiral mechanical forces, generated by the actomyosin cortex, play an important role in the left-right symmetry breaking. Confocal imaging, however, requires a gentle flattening of the embryo to allow for a full three-dimensional assessment of the embryo. Yet, even a gentle squeezing of the embryo can already delay cell divisions and subsequently lead to altered cell positions, suggesting that also the symmetry-breaking action of the actomyosin cortex can be affected. Using a custom-made lightsheet microscope that does not require any squeezing of the embryo, we have monitored actomyosin flows in the early embryo in three dimensions over time. Preliminary data from these experiments suggest that the previously observed chiral forces are even enhanced under these unconfined conditions.

BP 28.8 Thu 18:00 P2/EG

Organelle organization and dynamics in cells on soft substrates — •Paula Girones Paya, Florian Rehfeldt, and Matthias Weiss — Experimental Physics I, University of Bayreuth, Germany

The interior of eukaryotic cells features a highly organized and dynamically evolving set of compartments (organelles), e.g. mitochondria, the endoplasmic reticulum, or the nucleus. How these organelles self-organize to arrive at an arrangement that is beneficial for a cell is still poorly understood. Numerous studies have monitored organelle morphologies and dynamics in well-characterized culture cells grown on rigid substrates, e.g. glass coverslips. In real life, however, cells are situated in soft tissues with an elastic modulus that is five to six orders of magnitude lower. On soft substrates, actin-based stress fibers are less pronounced, and consequently cell morphologies are considerably less flattened by tensile forces, suggesting that also organelle arrangement and dynamics is altered. Here, we compare results of mitochondrial dynamics, cell nucleus volumes, and the exchange kinetics for diffusively driven transport between the nucleoplasm and the cytoplasm of cells on soft and rigid substrates.

BP 28.9 Thu 18:00 P2/EG

Quantifying Molecular Mobility, Abundance and Interactions by Fluorescence Correlation Spectroscopy — •Jana Sütterlin[1], Katharina Reglinski[1,2,3], Francisco Páez Larios[1,2], and Christian Eggeling[1,2] — [1]Institut für angewandte Optik und Biophysik, Friedrich-Schiller Universität Jena, Jena, Deutschland — [2]Leibnitz-Institut für photonische Technologien e.V., Jena, Deutschland — [3]Universitätsklinikung Jena, Jena, Deutschland

Since many biological functions rely on molecular interactions, knowledge about molecular mobility and diffusional processes are key to understand cellular signalling. To gain the desired insights, it is of utmost importance to develop and apply live-cell compatible approaches for diffusional investigations. Fluorescence Correlation Spectroscopy (FCS) is a powerful technique that enables the quantification of these dynamics.

This poster will provide an outline on how to utilise parameters acquired from FCS and dual-colour Fluorescence Cross-Correlation Spectroscopy (DC-FCCS) to quantify diffusion characteristics of particles in aqueous environments. This way, an examination of diffusional behaviour influenced by various binding conditions can be carried out.

FCS study about the peroxisomal import receptor PEX5 in live HEK cells is shown to elucidate its molecular interaction dynamics within the cytosol. Thereby the potential of FCS is exploited, highlighting its non-invasive, live-cell compatible properties. Ensuring proper function of organelles and cells, PEX5 transports cargo proteins featuring a targeting sequence, which need to be imported into peroxisomes.

BP 28.10 Thu 18:00 P2/EG

Evolution of the crowded state of cells as seen by FRET — •Avijit Kundu and Mattias Weiss — Experimentalphysik I, Universität Bayreuth, Universitätsstraße 30 95447 Bayreuth

Cells are the basic units of all living organisms. Somewhat surprisingly, however, virtually all cells feature very similar and high degrees of macromolecular crowding, with total concentrations of more than 100 mg/ml, irrespective of the species from which the cell is taken. Macromolecular crowding plays a key role in many biophysical processes and it can even alter biochemical cues by changing the binding kinetics or the steady-state frunction of associated states, suggesting that cells need to actively maintain their crowding state. Using a FRET sensor that reports on the local crowdedness in living cells, we have explored how individual cells can re-adapt their crowding state after a perturbation. Using a stepwise change of the osmotic pressure, we find that cells react rapidly to the external perturbation but aim at a relaxation back to the native state over time scales of minutes to hours.

BP 28.11 Thu 18:00 P2/EG

3D light-sheet microscopy of contracting skeletal muscle tissue — •Laura Strampe, Arne Hofemeier, Paul Maier, Jan Huisken, and Timo Betz — Third Institute of Physics - Biophysics, Georg August Universität, Göttingen

Skeletal muscle makes up the majority of human muscle tissue. Its contraction allows for controlled movements of the body, as well as being essential for maintaining posture. To understand the global and local forces at play during such contractions, occurring on the time scale of seconds, a 3D high-speed, high-resolution imaging method is necessary. We present a protocol for raising biomimetic muscle tissue anchored between two flexible mm-sized post. A full contraction cycle can be recorded through the synchronization of periodic electric stimuli and image acquisition using a custom build Flamingo light-sheet microscope. This enables us to study a wide range of questions including the influence of local contractile forces on muscle stem cell activation and contractile sarcomere dynamics.

BP 28.12 Thu 18:00 P2/EG

Screening for Pharmacologically Enhanced Tissues for Optical Microscopy. — •Venkat Raghavan Krishnaswamy, Susan Wagner, Rico Barsacchi, and Moritz Kreysing — Max Planck Institute of Molecular Cell Biology and Genetics. Dresden. Germany.

Our ability to observe the complexity of a living tissue under a light microscope is heavily impeded by the inherent light-scattering properties of the biological tissues. But remarkably some living tissues are highly transparent in nature, e.g., human retina, certain deep-sea creatures, etc. Comprehending and replicating the mechanisms by which tissue transparency is attained would unleash the full capabilities of optical microscopes. Here, we propose to unravel the molecular basis of tissue transparency in three-dimensional tissues using the immense potential of high-throughput screening and large-content image analysis tools. Specifically, we used active pharmacological compounds to screen for pathways that impact light-scattering properties in spheroids of human colorectal carcinoma cell line (HCT116). Randomly integrated multi-fluorescent beads within the spheroids served as an extrinsic readout factor and a conventional chemical-based clearing method was used as a positive control for assessing the optical properties of the tissue. The image analysis pipeline constructed to measure the intensities of the beads through the Z-sections clearly distinguishes cleared from uncleared spheroids. Overall, a robust assay was developed which would be employed on larger screens, to rapidly identify compounds and, further, signaling pathways that regulate the molecular mechanisms of tissue transparency.

BP 28.13 Thu 18:00 P2/EG

Imaging of vital mitochondria using Scanning Ion Conductance Microscopy (SICM) and electron microscopy methods

— •Eric Lieberwirth[1], Christian Völkner[1], Regina Lange[1], Anja Schaeper[2], Magdalena Otte[2], Marcus Frank[3], Kevin Oldenburg[4], Ingo Barke[1], Simone Baltrusch[2], and Sylvia Speller[1] — [1]University of Rostock, Institute of Physics — [2]Rostock University Medical Center, Institute for Medical Biochemistry and Molecular Biology — [3]Rostock University Medical Center, Medical Biology and Electron Microscopy Center — [4]University of Rostock, Center for Interdisciplinary Electron Microscopy MV

Mitochondria are enclosed by a double membrane. While the inner membrane with many insertions creates a large surface for the respiratory chain complexes, the outer one mediates fusion, fission and degradation of the organelles in the network. In this process, pole-like interaction sites develop, which impact the surface of the outer membrane. Scanning Ion Conductance Microscopy (SICM) allows the outer membrane of immobilized vital mitochondria to be measured in a buffer solution with a spatial resolution of about 50 nm and a height resolution of a few nanometers. The outer membrane shows dynamic height fluctuations as well as spatial height variations depending on the medium. Transmembrane proteins can be made visible when labelled with nanoscopic gold particles. A complementary study of SICM topographies, Scanning Electron Microscopy (SEM) and in situ liquid Transmission Electron Microscopy (TEM) images gives insight into the spatial distribution of internal and membrane-bound structures.

BP 28.14 Thu 18:00 P2/EG

Imaging Soft-Landed DNA-Aggregates — •Isabelle Legge, Jovana Pepic, Tim Esser, Márkó Grabarics, and Stephan Rauschenbach — Department of Chemistry, University of Oxford, Oxford, United Kingdom

Deoxyribose nucleic acid (DNA) is involved in important biological processes including replication, encoding information and gene expression. The helical structure of DNA double strands is well known but the superstructure of more complex assemblies such as DNA origami can be challenging to characterise by averaging techniques. Therefore, a versatile, yet practical, sample preparation technique is needed to make DNA-based molecules accessible to high-resolution, single-molecule imaging by atomic force microscopy (AFM) or transmission electron microscopy (TEM). Here, we use electrospray ion-beam deposition (ESIBD) to produce clean samples of single- and double-stranded DNA or DNA origami to enable AFM and TEM imaging, providing information on structure, conformation and revealing the mechanical properties. We discuss the advantages and limitations of this approach to improve the understanding of the function of these molecules.

BP 28.15 Thu 18:00 P2/EG

A backward-mode optical-resolution photoacoustic microscope for functional 3D imaging — •Elisabeth Baumann[1,2], Ulrike Pohle[3], Thomas Allen[4], Holger Gerhardt[1,2], and Jan Laufer[3] — [1]MDC, Berlin, DE — [2]Charite, Berlin, DE — [3]MLU, Halle, DE — [4]UCL, London, UK

Optical-resolution photoacoustic microscopy (OR-PAM) is a biomedical imaging technique with great potential for preclinical studies of the vasculature. It can be used to obtain spatially resolved information on parameters like the blood flow speed and blood oxygen saturation. However, for many in vivo applications, backward-mode operation of the OR-PAM system is required for which conventional piezoelectric ultrasound sensors are at a disadvantage as they need to be placed far away from the signal source. Here, we present an all-optical, backward-mode OR-PAM system that fulfils the requirements for functional imaging of the vasculature. The system incorporates a novel planar Fabry-Pérot (FP) ultrasound sensor, which is transparent to the excitation light and can be placed immediately adjacent to the sample.

To demonstrate the morphological imaging capabilities of the system, we performed 3D imaging in vitro of a leaf skeleton phantom and in vivo of a zebrafish embryo in raster-scanning mode. To be able to resolve blood flow, a fast continuous-scanning mode was established and validated in imaging phantoms. To show the capabilities of the system to image blood oxygen saturation, a Raman laser was set up for multi-wavelength excitation OR-PAM of ink phantoms.

BP 28.16 Thu 18:00 P2/EG

Imaging Symmetry-Dependent Behavior of Orbital Angular Momentum Entangled States — •Juan Nicolas Claro Rodriguez[1,2] and Roberto Ramirez Alarcon[1] — [1]Centro de Investigaciones en Óptica, 37150 León-Guanajuato, México — [2]Paderborn University, 33098 Germany

Orbital angular momentum (OAM) is a degree of freedom of photons, promising for many high-dimensional quantum applications. By tuning the symmetry of OAM states using dove prisms and measuring spatially resolved interference properties, we find that fringes are produced depending on the type of the state symmetry and propose an application to achieve twice the contrast in quantum optical coherence tomography. This technique also permits high-resolution microscopy of photo-sensitive tissue.

BP 28.17 Thu 18:00 P2/EG

Quantitative imaging of Caenorhabditis elegans dauer larvae during cryptobiotic transition — •Kyoohyun Kim[1], Vamshidhar R. Gade[2,3], Teymuras V. Kurzchalia[2], and Jochen Guck[1] — [1]Max Planck Institute for the Science of Light, Erlangen, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Institute of Biochemistry, ETH Zürich, Zürich, Switzerland

Caenorhabditis elegans can survive harsh environments by entering dauer diapause with reduced metabolic activity and distinct structural changes. We employed optical diffraction tomography (ODT) to quantitatively measure the transitions of mass density distribution inside living C. elegans larvae in the reproductive and diapause stages. ODT revealed that the mass density of C. elegans larvae increased upon entry into dauer diapause, and surprisingly, the harshly desiccated dauer larvae exhibited very high refractive index values (n ~ 1.5). Moreover, mutants that are sensitive to desiccation displayed structural abnormalities in the anhydrobiotic state that were not observable by conventional microscopy. Our findings open a door to quantitatively understanding the importance of material properties of an organism on the verge of life and death.

BP 28.18 Thu 18:00 P2/EG

Shaping the embyo: blastoderm stress maps reveal early mechanical symmetry breaking — •Alejandro Jurado Jiménez, Leon Lettermann, Bernhard Wallmeyer, and Timo Betz — Drittes Physikalisches Institut, Georg-August-Universität Göttingen

In this work we present a hydrodynamical analysis of early Zebrafish development which aims to understand the mechanical state of the tissue leading to its first symmetry breaking during epiboly: the shield formation. A full mechanical characterization of the blastoderm is achieved using a combination of Light-Sheet microscopy and state-of-the-art cell tracking of the cells nuclei, viscosity measurements and polyacrylamide beads as force sensors. The extraction of stress maps in the tissue is possible thanks to a custom-made software for the analysis of the bead deformation, which is presented here a versatile tool for similar stress analyses in other biological samples.

Our experimental analysis of the mechanical state of the embryo is supported and expanded by a model-driven extraction of the stress fields using NeuronalODEs. The NODEs system only necessitates the velocity field on the blastoderm to solve the hydrodynamic problem, optimizing up to 10^5 parameters and retrieving a full dynamical description of the embryo. Both the experimental and numerical analyses expose a stress asymmetry prior and during the shield formation, from which we can learn more about the mechanical origin of the first embryonal symmetry breaking.

BP 28.19 Thu 18:00 P2/EG

Radial growth and the impact of stress on the cell division plane in the hypocotyl — •Mathias Höfler and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

The morphogenesis of plant tissue is a reliably stable and efficient process, yet individual cell shape and growth underlie high variance. Theory and experiment show that there is a mechanical and biochemical feedback loop for plant tissue development. In fact, mechanical stresses have a pronounced effect on microtubule orientation in the tissue, thereby changing the mechanical properties and leading to anisotropic cell growth. Here, we study the effect of cell mechanics, stress patterns and feedback mechanisms on the bidirectional radial growth of the plant hypocotyl. We furthermore study the connection between mechanical stresses and the choice of cell division plane orientation. We seek to unveil the minimal biophysical requirements and relevant forces to achieve the experimentally observed morphologies. Our results show that inhomogeneous growth generates distinct stress patterns in the tissue . Introducing cell division along the direction of maximum stress furthermore gives us a first perspective on how radial growth morphologies emerge.

BP 28.20 Thu 18:00 P2/EG

3D Traction Force Microscopy on engineered blood vessels — •Karim Ajmail, Fatemeh Mirzapour, and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

The endothelium lines the walls of every blood vessel the human body. By virtue of their strategic position the endothelium has to withstand a plethora of mechanical cues including shear stress, circumferential strain as well as pressure exerted by the blood flow. Therefore, the mechanobiology of endothelial cells is a particularly pivotal part for the functionality of this tissue. However, the immense complexity of the vasculature necessitates in vitro systems that can uncouple and measure these various effects. Although in vitro approaches greatly enhanced our understanding of endothelial complexity, a mechanical characterization of endothelial systems is missing so far. Here, we employ 3D Traction Force Microscopy (TFM) as state-of-the-art method to measure cellular forces in physiologically relevant environments. In particular, we use 3D TFM to measure forces in a perfusable engineered blood vessel embedded in a fibrin hydrogel. Further, the effect of different stationary as well as pulsatile flow patterns on the mechanical response of the cells is investigated. We propose 3D TFM as an additional readout parameter in future human-on-a-chip applications for a quantitative mechanical characterization of the tissue.

BP 28.21 Thu 18:00 P2/EG

Tissue tension during zebrafish development — •Ming Hong Lui[1,2], Alejandro Jurado[1], Leon Lettermann[1,3], and Timo Betz[1,2] — [1]3rd Institute of Physics - Biophysics, University of Göttingen — [2]Max Planck School Matter to Life — [3]Institute for Theoretical Physics, Heidelberg University

Understanding the morphogenesis during development is one of the emerging fields where the interaction between developmental and tissue biology with biophysics has provided a series of new insights into nature's physical working principles. In particular, during embryonic development of zebrafish, cells in the blastoderm exhibit collective migration towards the yolk in a process known as epiboly, while simultaneously shield formation and gastrulation break symmetry preceding tissue differentiation. These elegantly robust processes are facilitated by both biochemical and mechanical interactions.

To determine how mechanical tissue stresses contribute to these interactions, we use photoablation to externally break symmetry by severing connections in the enveloping layer and record the subsequent population redistribution using light sheet microscopy of the whole embryonic volume. From the analysis of the nuclei trajectories, we noted that the epiboly process is highly robust and mostly unaffected by the damage, during which there is a convergent motion of cells towards an azimuthal angle (orthogonal to the direction of epiboly) that forms the future spine. Ablations can transiently disrupt this convergence dependent on the developmental time at which the damage is introduced.

BP 28.22 Thu 18:00 P2/EG

A 3D Voronoi vertex model for fluid transport in lumenogenesis — •Anne Materne[1], Charlie Duclut[1,2], Quentin Vagne[1,3,4], Pietro Incardona[3,5,6], Ivo F. Sbalzarini[3,5,7,8], and Frank Jülicher[1,3,8] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Laboratoire Physico-Chimie Curie, Paris, France — [3]Center for Systems Biology Dresden, Germany — [4]Department of Genetics and Evolution, Université de Genève, Switzerland — [5]Faculty of Computer Science, TU Dresden, Germany — [6]Institute for Genomic Statistics and Bioinformatics, Universität Bonn, Germany — [7]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [8]Cluster of Excellence Physics of Life, TU Dresden, Germany

In many systems, cells collectively organise to build complex structures. In particular, in certain developmental processes the formation of a fluid-filled cavity called a lumen plays a crucial role. Various mechanisms, for example programmed cell death, are known to initiate lumen formation. However, in order to sustain lumenogenesis, cells must collectively transport water and ions into the newly forming cavity. Here, we present a 3D Voronoi vertex model to study this collective transport process at cellular resolution. Our approach involves a substantial extension of the typical Voronoi work function minimisation procedures to account for the hydraulic and mechanical mechanisms in cell volume regulation and for pressure-driven flows. Fully-parallelised and efficient for systems with many cells, our procedure allows us to study the dynamics of lumenogenesis in complex geometries.

BP 28.23 Thu 18:00 P2/EG

Dystrophin as a tension regulator in human skeletal muscles — •Mariam Ristau[1], Arne Hofemeier[1,2], and Timo Betz[1] — [1]Third Institute of Physics - Biophysics, Georg-August-University Göttingen, Germany — [2]ZMBE - Institute of Cell Biology, University of Münster, Germany

Skeletal muscles are associated with contraction, movement and force generation. They are important for maintaining posture and maintaining bone and joint stability. Muscular dystrophies such as Duchenne muscular dystrophy (DMD) result in progressive weakening of skeletal muscles. DMD is caused by the loss of the protein dystrophin which is thought to stabilize and protect muscle fibers from injury. In the progression of the disease, damaged muscle fibers degrade, muscle mass is lost and greater functional impairments develop. We have studied the contractile potential of myoblasts and reconstituted tissue derived from healthy and DMD patients, and found that they were mechanically different in muscle tension and contractility. DMD derived myoblasts exhibited an overall weaker contractility compared to healthy derived myoblasts. In contrast, DMD derived myoblasts showed an overall higher muscle tension, suggesting that dystrophin may function as a tension regulator in skeletal muscles. In order to rule out the possibility that these findings are due to patient variability we intend to establish a genetic model in which we knockout dystrophin with the CRISPR/Cas9 system in healthy myoblasts and rescue dystrophin in DMD myoblasts by integrating micro-dystrophins(μDys).

BP 28.24 Thu 18:00 P2/EG

Influence of vimentin intermediate filaments on microtubules in cells — •Anna Blob[1], Roman David Ventzke[1,2], Thomas Giacomo Nies[2], Axel Munk[2], Laura Schaedel[3], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen — [2]Institute for Mathematical Stochastics, University of Göttingen — [3]Center for Biophysics, Saarland University

The cytoskeleton in eucaryotic cells is an intricate network of three different filamentous proteins: microtubules, actin filaments and intermediate filaments. They are essential for the mechanical properties of a cell as well as intracellular transport and division. Each filament type has its own unique features, and, in particular, microtubules, can withstand large compressive forces and show characteristic buckling and bending behavior that is still not fully understood. There is evidence for important interactions between cytoskeletal filaments: vimentin intermediate filaments stabilize microtubules in vitro and can template the microtubule network in migrating cells. Following up on this idea, we are interested in the influence of vimentin networks on microtubule mechanics. Investigating how the bending of microtubules depends on both the microtubule network itself and the vimentin network will improve our understanding of the mechanical consequences of the interaction within and between these filament systems. We compare microtubule networks in vimentin-knockout and wildtype mouse fibroblasts on micropatterns. We find that the local curvature of microtubules depends on the cellular region and increases with both increasing microtubule density and increasing vimentin density.

BP 28.25 Thu 18:00 P2/EG

Interactions between synaptic vesicles and cytoskeletal filaments — •Tiago Mimoso, Tizian Schmidt, and Sarah Köster — Institute for X-Ray Physics, University of Göttingen, Germany

Signal transmission of neurons occurs both electrically and chemically. The chemical signal is transported by synaptic vesicles(SVs) from one cell to another via the synaptic cleft to the adjacent neuron. Thus, these SVs are found in the synapse, within the so-called synaptic bouton. Here, the SVs are surrounded by cytoskeletal filaments, including dynamic microtubules that undergo rapid assembly and disassembly. There are studies that suggest an interactions between SVs and the cytoskeletal filaments, however the exact mechanisms remain unknown. Therefore, we now ask the question of whether SVs and microtubules interact and what influence the presence of SVs has on the growth rate, disassembly rate, catastrophe frequency and rescue frequency of the microtubules. We employ a reconstituted *in vitro* system and image the dynamic microtubules by total internal reflection fluorescence (TIRF) microscopy. We use a novel and fast data analysis technique based on a neural network to segment the microtubules in the microscopy pictures. This method provides the advantage of being applicable also curved microtubules and yields results that are comparable to the commonly used manual analysis method.

BP 28.26 Thu 18:00 P2/EG

Burst Mode Characteristics of an Ultrasonic Transducer for Treatment of Cancer Cells — •Rebecca Kampmann[1], Birte Sehlmeyer[1], Claus Scheidemann[2], Tobias Hemsel[2], and Mathias Getzlaff[1] — [1]Institute of Applied Physics, Düsseldorf University — [2]Dynamics and Mechatronics, Paderborn University

Head and neck squamous cell carcinoma cells and oral keratinocytes have different cell mechanics and because of that they have different natural frequencies. This characteristic is used to selectively destroy cancer cells.

For this purpose, ultrasonic waves at a resonant frequency of 90kHz were used in burst mode to achieve the largest possible deflection of the ultrasonic transducer. The ultrasonic actuators were electrically excited using a flexible ultrasonic generator developed by ATHENA Technologie Beratung GmbH, Paderborn. Investigation of the active current, which is proportional to the transducer tip velocity, showed that the active current depends on the set active time. If the active time is too low, the active current is not able to reach the desired target current. The longitudinal deflection of the ultrasonic probe in burst mode is comparable to the one in continuous mode. The set-point current amplitude and the active time are decisive parameters. In addition, the transverse deflection was investigated, showing that this vibration is larger than the longitudinal one.

BP 28.27 Thu 18:00 P2/EG

Burst Mode of Ultrasonic Resonant Oscillations for Stimulation and Destruction of Tumor Cells — •Birte Sehlmeyer[1], Rebecca Kampmann[1], Claus Scheidemann[2], Tobias Hemsel[2], and Mathias Getzlaff[1] — [1]Applied Physics, Düsseldorf University — [2]Dynamics and Mechatronics, Paderborn University

Different types of cancer, such as prostate carcinomas, are nowadays already treated with the ultrasound-based therapy HIFU (high intensity focused ultrasound). The healthy cells, which are located in the irradiation field, cannot be spared in this process. The elasticity differences between cancer cells and healthy cells strongly influence their stimulation frequency. LIPUS (low intensity pulsed ultrasound) is used to selectively stimulate and destroy cancer cells close to their own natural frequency, while sparing locally adjacent healthy cells.

Here we report new findings on the maximum oscillation amplitude of an ultrasound unit in burst mode. In burst mode, there is only a signal output during the active times.The ultrasonic actuators were electrically excited using a flexible ultrasonic generator developed by ATHENA Technologie Beratung GmbH, Paderborn. The excitation of the ultrasonic unit was varied by setting the targets current amplitude and the active time. Regarding the characteristic stimulation frequency of tumor cells, the frequency spectrum and frequency filters are discussed. In addition to the longitudinal deflection amplitude, an oscillation in the transverse direction was observed. Finally, the transverse oscillation behavior is investigated in relation to half-wave synthesis.

BP 28.28 Thu 18:00 P2/EG

Cytoskeletal Networks in Cells Under Strain — •Ruth Meyer[1], Anna V. Schepers[1], Peter Luley[1], Jonathan Bodenschatz[2], Amaury Perez Tirado[2], Andreas Janshoff[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen — [2]Institute for Physical Chemistry, University of Göttingen

The cytoskeleton of eukaryotes consists of three types of filaments: F-actin, microtubules and intermediate filaments (IFs). In contrast to microtubules and actin filaments, IFs are expressed in a cell-type specific manner, and keratins are found in epithelial cells. In certain cell types, the keratin filaments form a layer close to the membrane which may be referred to as an "IF-cortex". Furthermore, it is hypothesized that this IF-cortex arranges with radial spokes in a "rim-and-spokes" structure in epithelia. Based on this hypothesis, IFs and actin filaments might add complementary mechanical properties to the cortex. It was previously shown that single IFs remain undamaged even at high strains. We now ask the question of whether this unique force-extension behavior of single IFs is also relevant in the filament network within a cell. We designed an equibiaxial stretcher that can apply high strains to the cells. This setup is combined with fluorescence and atomic force microscopy enabling simultaneously imaging of the cells and measuring their stiffness during stretching. By quantitatively analyzing the force indentation curves and the microscopy images, we analyze the structure and the mechanical properties of actin and IF networks close to the cell membrane.

BP 28.29 Thu 18:00 P2/EG

Exploring cell-cell interactions inferred from trajectories in two-site arrays — •Emily Brieger[1], Tom Brandstätter[2], Georg Ladurner[1], Chase P. Broedersz[2], and Joachim O. Rädler[1] — [1]LMU, Munich, Germany — [2]VU Amsterdam, Amsterdam, Netherlands

Collective cell migration is a fundamental aspect to a variety of physiological processes. The migratory dynamics of these collective processes rely on cell-cell interactions that are depending on complex molecular mechanisms, such as cadherin dependent pathways. In previous work we studied the interaction behavior of two cells migrating on dumbbell-like micropattern. This geometry enforces repeated head-to-head collisions of cells and allows the distinction of interacting and noninteracting events. In this framework non-cancerous MCF10A cells and cancerous MDA-MB-231 cells clearly differ in their effective adhesion and friction terms derived from quantitative theoretical analysis. Here we use this data-driven approach to study how specific molecular alterations of surface proteins change cell-cell interactions in different cell lines. Blocking of E-cadherin and Ephrin A2 via antibodies yield distinct shifts in cell behavior space. Likewise knockouts that prevent cells from using their usual communication pathways alter the adhesive and frictional interactions. We show that the analysis yields insight into the role of E-Cadherin and Ephrin A2 in frictional and adhesive interactions as well as repulsive response known as contact inhibition of locomotion.

BP 28.30 Thu 18:00 P2/EG

A high-throughput pipeline for morphological and functional analysis of cardiomyocytes — Daniel Härtter[1,2], •Lara Hauke[1], Wolfram-Hubertus Zimmermann[1], and Christoph F. Schmidt[2] — [1]Institute of Pharmacology and Toxicology, University University Medical Center Göttingen, Germany — [2]Department of Physics, Duke University, Durham, NC, USA

Cardiomyopathies, diseases of the heart muscle, affect 1 in 500 adults in Western countries. Nevertheless, reliable knowledge about disease onset and pathogenesis is lacking. To develop effective treatment options for patients, a dynamic and quantitative understanding of cardiomyopathies is needed. We developed an assay in which individual stem-cell derived heart cells of a fluorescent sarcomere reporter cell line grow in a heart-like environment - while allowing for automated high-resolution and high-framerate imaging - using micropatterned polyacrylamide acid (PAA) gels. We analyze the time-course of cell morphology and function upon drug-induced or genetic interventions with our deep-learning-based SarcAsM (Sarcomere Analysis Multitool) software. The resulting multiparametric functional and structural trajectories of cardiac muscle cells can be used to gain novel dynamical perspectives on the time-course and interplay of structure and function in health and disease and might contribute to the discovery of novel treatments.

BP 28.31 Thu 18:00 P2/EG

A mechanical bottom-up approach of memory formation in *Physarum polycephalum* — •Mathieu Le Verge Serandour and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

Understanding the emergence of memory in artificial or living complex systems is a considerable challenge: its origin, possibly an interplay of physics, genetics, or signaling, has not yet been elucidated. *Physarum polycephalum*, a unicellular organized as a two-dimensional tubular network, exhibits hallmarks of memory formation: its adaptive morphology encodes the location of past stimuli. We propose to investigate memory formation with a bottom-up approach focusing on the physical mechanisms of vascular morphology adaptation. First, we study the mechanical properties of *Physarum* by microrheology. We measure the viscoelasticity of the network's tubes and protrusions, and the change in stiffness or viscosity exposed to external stimuli, such as light or food. At the macroscopic scale, we study the dynamics of pruning of the network and its remodeling. We find an exponential decrease in the number of tubes reproduced by a toy model based on network hierarchy. These two complementary approaches will allow us to build a solid basis for establishing physical principles to characterize information encoding and memory emergence in *Physarum polycephalum*.

BP 28.32 Thu 18:00 P2/EG

Viscoelastic response of vimentin intermediate filament networks measured via optical tweezers-based active microrheology — •Kaan Ürgüp[1], Anna V. Schepers[2], and Sarah Köster[1]

— [1]Institute for X-Ray Physics, Universität Göttingen, Germany — [2]Rosalind Franklin Institute and Kennedy Institute of Rheumatology, University of Oxford, UK

The microscale mechanics of the intermediate filament (IF) cytoskeleton are relevant for many cellular processes. The properties of the IF network have been shown to influence cell motility, migration and organelle transport. On the molecular level, an IF monomer is composed of amino acids that lead to α-helical domains in the center, flanked by non-helical domains. Multiple monomers assemble laterally to unit-length-filaments and longitudinally to mature filaments. Vimentin is the most abundant IF protein in humans. Single vimentin filaments show a loading-rate dependent behavior, which can be attributed to the unfolding of α-helical structures into disordered structures and β-sheets when high strains are applied. What is unclear, however, is whether this nonlinear behavior is relevant in cellular vimentin networks. In this work, we measure strain and relaxation dynamics of *in vitro* vimentin networks via optical tweezers in the nonlinear regime. We use an active-passive calibration method based on the Onsager theorem. We measure the nonlinear response to different oscillation amplitudes, which correspond to different strains applied to the network. Our setup allows us to investigate whether the nonlinear behavior of the single filaments is preserved on the network scale.

BP 28.33 Thu 18:00 P2/EG

Traction force microscopy quantifies the contractility of laminopathic cardiomyocytes — •Valentina Kuhn[1,2], Christina Goss[1,3], Aiste Liutkute[2], Anna Zelena[1], Ulrich S. Schwarz[3], Niels Voigt[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen, Germany — [2]Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Germany — [3]Institute for Theoretical Physics, University of Heidelberg, Germany

Cardiomyocytes generate the contractile forces in the intact heart. In their nuclear lamina, cardiomyocytes express lamins A and C, a type of intermediate filament proteins that are encoded by the *LMNA* gene and are important for both genetic regulation and cytoskeletal organization. Patients with pathogenic *LMNA* mutations typically suffer from diseases characterized by altered cardiomyocyte contractile behavior, leading to high sudden cardiac death rates. So far, no detailed mechanistic explanation nor specific therapies are available. Cardiomyocytes derived from induced pluripotent stem cells (iPSC-CMs) are powerful in-vitro models to study the mechanisms underlying cardiomyopathies. We combine traction force microscopy with fluorescence imaging of the actin structures in a time-resolved manner on a single cell level. The experiment is conducted by seeding iPSC-CMs on elastic substrates featuring fibronectin micropatterns, which regularize their geometry for imaging while simulating physiological conditions. Thus, we can quantify the altered contractility of iPSC-CMs with the R331Q *LMNA* mutation in comparison with wild-type cells.

BP 28.34 Thu 18:00 P2/EG

Cell migration on micropatterns - how regular is the motion of different cell types? — •Annika A. Vogler, Sebastian W. Krauss, Radhakrishnan A. Veettil, Florian Rehfeldt, and Matthias Weiss — Experimental Physics I, University of Bayreuth, Germany

During processes like embryonic development, wound healing, or cancer metastasis, cells are often migrating in complex and obstacle-rich environments. Microstructured surfaces offer a versatile opportunity to model such environments and study cell migration under controlled conditions. Recent studies on cells that migrate in fairly simple two-state micropatterns have revealed, for example, a rich and nonlinear migration dynamics [1]. Following up on this study, we have explored the migration dynamics of non-cancerous MCF-12A cells on simple dumbbell patterns in comparison to malignant MDA-MB-231 cells. As a result, we observed that MCF-12A cells exhibit a strikingly more regular migration pattern while trajectories of cancerous cells appeared more stochastic. In particular, the path of non-tumorigenic cells was mainly focused on the edges of the pattern whereas malignant cells explored the whole available adhesion area. These results suggest differences in how the external environment is perceived by the internal biochemical state of cells.

[1] Brueckner, Fink, Schreiber et al., Nat. Phys. 15, 595 (2019)

BP 28.35 Thu 18:00 P2/EG

Cell Shape and Tension alter Focal Adhesion Structure — Carolin Grandy[1], Fabian Port[1], •Jonas Pfeil[1], Mariana Azevedo Gonzalez Oliva[2], Massimo Vassalli[2], and Kay-Eberhard Gottschalk[1] — [1]Universität Ulm, Institut für experimentelle Physik, Ulm, Germany — [2]University of Glasgow, James Watt School of Engineering, Glasgow, United Kingdom

Cells are anchored to the extracellular matrix via the focal adhesion complex. It also serves as a sensor for force transduction. We analyse the effect of tension on the location of key focal adhesion proteins vinculin, paxillin and actin. We use micropatterning on gold surfaces to manipulate the cell shape, to create focal adhesions at specific cell areas, and to perform metal-induced energy transfer (MIET) measurements on the patterned cells. We use drugs influencing the cellular motor protein myosin or mechanosensitive ion channels to get deeper insight into focal adhesions at different tension states. We show here that in particular actin is affected by the rationally tuned force balance. Blocking mechanosensitive ion channels has a particularly high influence on the actin and focal adhesion architecture, resulting in larger focal adhesions with elevated paxillin and vinculin and strongly lowered actin stress fibres. Our results can be explained by a balance of adhesion tension with cellular tension together with ion channel-controlled focal adhesion homeostasis, where high cellular tension leads to an elevation of vinculin and actin, while high adhesion tension lowers these proteins.

BP 28.36 Thu 18:00 P2/EG

Interactions of cytoskeletal elements during phagocytosis in macrophages. — •Erbara Gjana[1] and Franziska Lautenschläger[1,2] — [1]Department of Physics, Saarland University, Saarbrücken, Germany — [2]Center for Physics, Saarland University, Saarbrücken, Germany

The structure of cells is realized via their cytoskeleton - a polymer network inside cells. It is the main component of structural integrity and it shapes cells. The cytoskeleton is involved in many active cellular activities that includes cell division, migration, and phagocytosis. In macrophages, we know that actin - one protein of the cytoskeleton * plays an important role during phagocytosis. In my project, I work on understanding how actin is involved in sensing the object which needs to be phagocytosed.

Particularly, I study the effect of the physical properties such as form, size and stiffness of the objects. Therefore, I am varying the stiffness of objects, e.g. I use gelatine beads, latex beads and polystyrene beads and investigate how these are phagocytosed with the help of actin. Through different microscopy methods (epi-fluorescence, confocal) I will be able to image the process of phagocytosis. Till now, we have established phagocytosis protocols with macrophages derived from the cell line HL60. For a better biological fit I am now shifting to THP1 derived macrophages. This will help me to understand questions such as how macrophages distinguish between dead cells (ei. Dead RBCs), cell debris, and healthy cells. Also, we collaborate with theoreticians be build general mathematical model of phagocytosis.

BP 28.37 Thu 18:00 P2/EG

Micromechanics of spherical cellular aggregates — •Antoine Girot[1,2], Marcin Makowski[2], Marco Rivetti[2], Christian Kreis[2], Alexandros Fragkopoulos[1,2], Matilda Backholm[3], and Oliver Bäumchen[1,2] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [3]Aalto University School of Science, Department of Applied Physics, 02150 Espoo, Finland

Understanding the rich dynamics of biophysical processes, such as pathogenic tissue development and morphogenesis, requires a proper mechanical characterization of multicellular aggregates. Spherical aggregates often serve as model systems, yet, they cannot be readily characterized with conventional techniques that are optimized for single cells. In this presentation, we report on *Volvox globator*, a natural cellular aggregate that is composed of hundreds of bi-flagellated cells forming a spherical monolayer filled with mucilage. We employ *in vivo* micropipette force measurements combined with optical detection to simultaneously measure the force response and the deformation of this living aggregate. We show that the micromechanics of *Volvox* can be described by a model coupling elasticity and viscosity, which allows to extract the mechanical properties. We find that the viscous component exhibits a shear-thinning behavior, that can be properly described by implementing a power-law fluid model, while the elasticity of the aggregate depends on its size.

BP 28.38 Thu 18:00 P2/EG

The influence of calcium on the structure of the actin cortex in cell monolayers and single cells — •Christoph Anton[1], Lucina Kainka[1], Sandra Iden[2], and Franziska Lautenschläger[1,3] — [1]Department of Physics, Saarland University, Saarbrücken, Germany — [2]Center of Human and Molecular Biology (ZHMB), Saarland University, Homburg, Germany — [3]Center for Biophysics, Saarland University, Saarbrücken, Germany

We recently showed that adhesion to a substrate, mediated via integrins, causes significant changes to the structure, mechanics and dynamics of the cellular actin cortex. In tissues, however, cells additionally form cell-cell junctions. Therefore, we investigate how the structure of the actin cortex of healthy and cancerous epithelial cell lines is affected by the transition from single cells to cell monolayers. One important step during this transition is the formation of cell-cell junctions, such as the cadherin-based adherens junctions. These junctions are dependent on the presence of calcium ions. In our work, we varied the extracellular calcium concentration to investigate the effect of cadherin-mediated adhesion and other calcium-based cellular processes on the actin cortex. We used scanning electron microscopy (SEM) to visualize the actin cortex. We applied our filament network tracing algorithm to the SEM images to quantify the structural properties of the actin cortex, such as the mesh hole area. By comparing the cortex parameters of cells within a monolayer with the cortex parameters of isolated cells we plan to characterize the structural changes that are induced by cell-cell contacts and extracellular calcium concentrations.

BP 28.39 Thu 18:00 P2/EG

Motility of adherent cells on structured surfaces at elevated viscosities — •Radhakrishnan Adiyodi Veettil, Sebastian W Krauss, Annika A Vogler, Florian Rehfeldt, and Matthias Weiss — Experimental Physics I, University of Bayreuth, Germany

Cell motility is sensitive to the viscosity of the surrounding medium, suggesting that such external cues can trigger cells to switch gears. Indeed, it has been recently reported that elevated viscosities can induce significant changes in cell area, cell migration speed and focal adhesion turn over [1]. Here, we have followed up on these experiments by monitoring the viscosity-dependent migration of different cell types on microstructured surfaces, e.g. cell hopping of cancerous and non-cancerous cells in dumbbell patterns. Our data suggest that altering viscosity can markedly alter the migration dynamics of cells on microstructured surfaces.

[1] Pittman, Iu, Li et al., Nat. Phys. 18, 1112 (2022)

BP 28.40 Thu 18:00 P2/EG

Coordination of information in *Physarum polycephalum* — •Kaspar Wachinger[1], Johnny Tong[1], Nico Schramma[2], Siyu Chen[1], and Karen Alim[1] — [1]School of Natural Sciences, Technical University of Munich, Germany — [2]Faculty of Science, University of Amsterdam, The Netherlands

Physarum polycephalum is a network-structured, single-cell organism with thousands of nuclei that can sense and adapt to its environment. To understand how *P. polyephalum* maintains efficient gene expression, it is necessary to understand the coordinated intracellular transport of nuclei within its structure. Microinjecting several fluorescent dsDNA markers into the tubes of *P. polyephalum* allows in-vivo imaging of nuclei and their dynamics: Nuclei can either be trapped in the more solid wall cortex or follow the oscillatory cytoplasmic streaming. We investigate the flow-driven behaviours of nuclei in functionally different regions of *P. polycephalum*'s network and motivate a hypothesis of inter-nuclei communication far past the degradation distance of mRNA.

BP 28.41 Thu 18:00 P2/EG

FilamentSensor 2.0: An open-source modular toolbox for 2D/3D cytoskeletal filament tracking — Lara Hauke[1], Andreas Primessnig[1], •Emese Zavodszky[1], and Florian Rehfeldt[2] — [1]Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Germany — [2]Experimental Physics I, University of Bayreuth, Germany

Cytoskeletal pattern formation and structural dynamics are key to a variety of biological functions and a detailed and quantitative analysis yields insight into finely tuned and well-balanced homeostasis and potential pathological alterations. High content life cell imaging of fluorescently labeled cytoskeletal elements under physiological conditions is nowadays state-of-the-art and can record time lapse data for detailed experimental studies. However, systematic quantification of structures and in particular the dynamics (i.e. frame-to-frame tracking) are essential. Here, an unbiased, quantitative, and robust analysis workflow that can be highly automatized is needed. For this purpose we upgraded and expanded our fiber detection algorithm FilamentSensor [1] to the FilamentSensor 2.0 [2] toolbox, allowing for automatic detection and segmentation of fibrous structures and the extraction of relevant data (center of mass, length, width, orientation, curvature) in real-time as well as tracking of these objects over time and cell event monitoring. Furthermore, we offer the Focal Adhesion Filament Cross-correlation Kit (FAFCK) [3] for automated correlation with point-like structures. [1] B. Eltzner, et al., PLoS One, 2015 [2] L. Hauke, et al., PLoS One, under review [3] L. Hauke, et al., PLoS One, 2021

BP 28.42 Thu 18:00 P2/EG

Mechanically induced Bioluminescence - from single cells to glowing sea — •Nico Schramma[1], Hugo França[1,2], and Maziyar Jalaal[1] — [1]Van der Waals-Zeeman Institute, University of Amsterdam, Amsterdam, Netherlands — [2]Instituto de Ciências Matemáticas e Computação, Universidade de São Paulo, São Carlos, Brazil

The ability of single-celled organisms to sense mechanical cues is of high importance for their migration, navigation and survival in their ever-changing environment. However, studying single-cell mechanosensing under dynamic mechanical conditions is complicated. For this reason, the bioluminescent marine algae Pyrocystis lunula is a particularly interesting organism: mechanical stimuli trigger them to release a flash of blue light, which is mostly known from the bioluminescent tide, turning the sea into a mysterious pale blue shimmering. Combining mechanical tests on single cells with dynamics of millions of bioluminescent algae in a wave impact experiment and computational fluid mechanics we find and test general relations describing macroscopic (fluid)mechanical cues with bioluminescence. Our research paves the way towards a better understanding of mechanosensation of algae and plants, but may also lead to applications of bioluminescent organisms as "living force sensors".

BP 28.43 Thu 18:00 P2/EG

Predicting optimal optogenetic control of cell migration with an active gel model — •Oliver M. Drozdowski, Falko Ziebert, and Ulrich S. Schwarz — Institute for Theoretical Physics and BioQuant, Heidelberg University, 69120 Heidelberg, Germany

Cell motility is one of the hallmarks of life and often results from flow in the actin cytoskeleton that is driven by actin polymerization at the front and myosin II motor contractility at the back. The standard model to describe such flows is active gel theory, in which myosin II contractility enters as active stress. Advancements in optogenetic tools have sparked interest in controlling these flows externally and consequently also motility.

Recently we have shown that bistability between motile and sessile states emerges in a one-dimensional active gel model if the myosin II motors are modeled as a supercritical van der Waals fluid [1]. We now incorporate optogenetic perturbations into this description and consider two experimentally accessible protocols for migration control - localized contractility perturbations and global upregulation of contraction. We find that the local protocol permits full external control. Global upregulation reliably leads to irreversible motility initiation, but does not allow for full control. Our results agree with recent experiments on cell migration in microchannels and reconcile experimental observations of local versus global regulatory mechanisms.

[1] O. M. Drozdowski, F. Ziebert, U. S. Schwarz, arXiv:2206.05915 (2022).

BP 28.44 Thu 18:00 P2/EG

Nuclei trafficking dynamics in Physarum polycephalum — •Johnny Tong, Kaspar Wachinger, Nico Schramma, and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

Synthetical organism and organs house up to thousands of nuclei within a single envelope, often shaped into a complex network architecture. How are nuclei able to efficiently exchange signals over long distances? To understand how synthetia coordinate gene expression, intracellular transport within these networks is key. Physarum polycephalum is an ideal syncytia model as its network-shaped body is a single multinucleated cell which can sense and adapt to its environment in a short time scale and a long length scale. Here, nuclei are trapped in the tube walls or advected by the oscillatory cytoplasmic streaming. We investigate its flow-driven dynamics and mechanochemical behaviors using image-based methods, including particle tracking

and velocimetry, to analyze the nuclei trafficking. We also utilize the thousands of nuclei to propose a new technique akin to traction force microscopy. By analyzing the fluctuations of nuclei trapped in the actomyosin cortex, we can probe the change of mechanical properties due to external stimuli, such as food, substrate stiffness, and light. Our techniques may be applied to other systems to unveil the mechanisms of long-range genetic communication within network-shaped organisms like fungi.

BP 28.45 Thu 18:00 P2/EG

Super-resolved Imaging of Cellular Traction Forces — •Armina Mortazavi, Jianfei Jian, and Benedikt Sabass — Ludwig Maximilian University of Munich, Munich, Germany

Traction force microscopy (TFM) is a well-established method that enables the measurement of forces that are exerted by adherent cells to an underlying substrate. We aim to enhance the spatial resolution of TFM by using stochastic optical reconstruction microscopy in total internal reflection mode. To measure the substrate deformations below adherent cells, we employ DNA-based FluoroCubes that each carries multiple, spontaneously blinking, fluorescent dye molecules. Grafting of these new fluorescent probes to the top surface of Polydimethylsiloxane gels and using RGD peptides as the smallest ligands representative of extracellular matrix allows us to measure the forces generated by individual focal adhesion sites. The proposed method in principle allows one to extend traction force microscopy to lengthscales below 100 micrometers and can therefore help to unravel the mechanobiology of highly localized cell-physiological processes.

BP 28.46 Thu 18:00 P2/EG

Length distributions of microtubles with a multistep catastrophe mechanism — Felix Schwietert, •Lina Heydenreich, and Jan Kierfeld — TU Dortmund University, 44227 Dortmund, Germany

Regarding the experimental observation that microtubule catastrophe can be described as a multistep process, we extend the Dogterom-Leibler model for dynamic instability in order to discuss the effect that such a multistep catastrophe mechanism has on the distribution of microtubule lengths in the two regimes of bounded and unbounded growth. We show that in the former case the steady state length distribution is non-exponential and has a lighter tail if multiple steps are required to undergo a catastrophe. If rescue events are possible, we detect a maximum in the distribution, i.e., the microtubule has a most probable length greater than zero. In the regime of unbounded growth, the length distribution converges to a Gaussian distribution whose variance decreases with the number of catastrophe steps. All results are verified by stochastic simulations.

BP 28.47 Thu 18:00 P2/EG

Bridging the gap between surface flows and motility patterns of malaria parasites — •Leon Lettermann[1], Mirko Singer[2], Falko Ziebert[1], Friedrich Frischknecht[2], and Ulrich S. Schwarz[1] — [1]ITP & Bioquant, Heidelberg University — [2]CIID, Heidelberg University

Malaria is one of the most devasting infectious diseases and transmitted from mosquitos to humans by so-called Plasmodium sporozoites, which move by gliding motility. Myosin motors move actin filaments below the plasma membrane, which leads to surface flows of adhesins that are anchored into the plasma membrane. How this surface flow is converted into the complicated motility patterns observed in experiments is not clear. Here we introduce a theoretical model that bridges this gap. The coupling between surface flow and substrate is modeled by a system of reversible adhesion bonds. We numerically solve the resulting system of ordinary differential equations and find a rich variety of motility patterns, including the circular and helical paths observed in experiments. This allows us to estimate likely patterns of surface flows, which are hard to measure experimentally.

BP 28.48 Thu 18:00 P2/EG

Stem Cell Dynamics in Tissues — •Johannes C. Krämer, Gerhard Gompper, and Jens Elgeti — Theoretical Physics of Living Matter (IBI-5/IAS-2), Forschungszentrum Jülich, Jülich, Germany

The renewal of epidermal tissue relies on a few stem cells dividing asymmetrically, and a cascade of transient amplifying cells resulting in the necessary cell mass of terminally differentiated cells. We integrated this process in the two-particle growth model, and find that this simple process results in very interesting dynamic features: Stem cells repel each other in the tissue bulk and are thus found rather isolated in the tissue.

Simulating just two isolated stem cells, we construct the probability density function to find two stem cells in a given distance, and observe a reduced probability to find stem cells close to each other. To understand this repulsive mechanism better, we apply equilibrium methods to construct an effective interaction potential. Although a massive simplification it allows us describe the repulsive interaction in a simple fashion. Thermal colloid simulations, where particles interact via the effective interaction, are consistent with simulations of bulk tissues.

Our findings may contribute to better understand the cancer stem cell hypothesis. Here, cancerous growth is assumed to emerge from few stem cell like cancer cells, which might evade being targeted by therapy. However, the cancer stem cells are difficult to observe – maybe because they get separated by this mechanism.

BP 28.49 Thu 18:00 P2/EG

On multistability and constitutive relations of cell motion on Fibronectin lanes — •Johannes Clemens Julius Heyn[1], Behnam Amiri[2], Christoph Schreiber[1], Martin Falcke[2,3], and Joachim Oskar Rädler[1] — [1]Ludwig-Maximilians-Universität München — [2]Max Delbrück Center for Molecular Medicine in the Helmholtz Association — [3]Humboldt Universität zu Berlin

Migration of eukaryotic cells is a fundamental process for embryonic development, wound healing, immune responses, and tumour metastasis. Experiments on 2d migration show a broad spectrum of morphodynamic features for many cell types. Cells exhibit distinct motile states: They are spread or moving and either steady or oscillatory and they display spontaneous transition between those states. Here, we present a study of the motion of MDA-MB-231 cells on 1d Fibronectin (FN) microlanes and group the migratory behaviour into four discrete states. A high-throughput setup allows to quantitatively analyse state transitions for a broad range of FN densities. We develop a biophysical model based on the force balance at the protrusion edge, the noisy clutch of retrograde flow and a response function to integrin signalling. The model reproduces cell states, characteristics of oscillations and state probabilities in very good agreement with our experimental data. The statistics of trajectories and theory suggests an adhesion related mechanism that not only explains multistability but also the well-known biphasic adhesion-velocity relation and the universal correlation between speed and persistence (UCSP).

BP 28.50 Thu 18:00 P2/EG

Single-molecule tracking in dense images — •Jianfei Jiang[1,2], Armina Mortazavi[1,2], and Benedikt Sabass[1,2] — [1]Institute for Infectious Diseases and Zoonoses, Department of Veterinary Sciences, LMU München — [2]Department of Physics, LMU München

Traction force microscopy (TFM) quantifies cellular traction forces on a surface. The technique is based on measuring the deformations in the substrate. A standard implementation of TFM involves using first particle image velocimetry (PIV) to measure the two-dimensional deformations. Subsequently, a force reconstruction algorithm calculates the traction field based on PIV measurements. The spatial resolution of TFM can be improved by using smaller-sized fluorescent particles embedded in the substrate. To this end, we develop a new technique that combines TFM with Stochastic Optical Reconstruction Microscopy (STORM). Using STORM, we can record the positions of FluoroCubes ($\sim$ 6nm) that are densely distributed in the substrate. Here, we propose a new single-molecule tracking algorithm to acquire fine-grained displacement fields. We first use PIV with large-sized fluorescent beads ($\sim$ 40nm) to obtain coarse-grained displacement fields, which helps us to estimate the displacement of each FluoroCube. Then, the tracking process is formulated as a linear assignment problem, where we implement the Hungarian algorithm to minimize the overall deviation from PIV estimations. The particle tracking algorithm is parallelized by dividing the image into smaller subimages to reduce computation time. The tracking results enable us to build a high-resolution displacement field for force reconstruction.

BP 28.51 Thu 18:00 P2/EG

Reconstituting a polymer hydrogel that mimics intracellular viscoelastic properties — •Dorian Marx, Bart Vos, and Timo Betz — 3. Institute of Physics, Faculty of Physics, Georg-August-University Göttingen

Throughout the years numerous models were developed that describe the mechanical response of cells to deformations. However, all models, both classic and modern, are phenomenological, that is, they lack

a connection of their parameters to the real physical system, making them hard to interpret. Furthermore, the strongest argument for a particular model so far is how accurately it matches to measurements. While this is fine on a phenomenological level, a deeper understanding, e. g. why it fits, is missing. This also holds for the fractional Kelvin-Voigt model (fKVM) that is composed of two complex power-laws and was shown to fit a range of different cells very well.

To connect the fit parameters of the fKVM to the physical system we opt for a bottom-up approach by using a passive viscoelastic polymer with constituents that have analogs in cells. After confirming that the fKVM accurately fits this system, we focus on finding "the most cell-like" parameter set. Varying the composition of the gel (e. g. via the cross-linker concentration) allows us to directly connect properties of the physical system to model parameters. With this, we are now able to formulate hypotheses that can be checked in live cells, giving a quantitative handle for connecting the real world biophysics to rheological models.

BP 28.52 Thu 18:00 P2/EG

Does Size Matter? Actin filament length in cell migration — •Carsten Alexander Baltes[1], Divyendu Goud Thalla[1], and Franziska Lautenschläger[1,2] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Center for Biophysics, Saarbrücken, Germany

The ability to perform cellular locomotion is crucial for a large variety of tasks. This includes the search and chase of immunecells for pathogens as well as the search for food and the reorganisation of cells in tissue developement. The cytoskeleton protein actin is particularly important for migration of eucaryotic cells. It is involved in the formation of filopodia and creates a retrograde flow from the leading edge towards the back of the cell, both of which allow them to move forward. Alteration of the actin network therefore might have an impact of the migratory behavior of cells. Here I am going to present the effects of elongated actin filaments on migrating RPE-1 cells. I will show that cells, migrating either on 1D fibronectin lines or on a fibronectin coated surface, displayed a reduction of migration speed, while keeping their persistence. They also occupy a larger area when allowed to spread freely and expres a higher amount of focal adhesions. The change in migration speed vanishes when we put those cells under confinement in PDMS microchannels. Taking those facts together we propose that the length of actin filaments is important for cell migration. However further research is needed to fully understand the importance regarding the different migration modes cells can take depending on the surrounding environment.

BP 28.53 Thu 18:00 P2/EG

From Shape to Function of Sampling Resident Tissue Macrophages — •Miriam Schnitzerlein[1], Anja Wegner[2], Stefan Uderhardt[2], and Vasily Zaburdaev[1] — [1]Department of Biology, Friedrich-Alexander-Universität Erlangen-Nürnberg and Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [2]Department of Internal Medicine 3 - Rheumatology and Immunology, Friedrich-Alexander-Universität Erlangen-Nürnberg und Universitätsklinikum Erlangen, Germany

Mammalian tissues are permanently subjected to various stresses - be it pathogens, dead cells and related waste products or injuries like micro-lesions - which have to be resolved properly to prevent inflammations and maintain tissue homeostasis. To detect such incidents, sessile resident-tissue macrophages (RTMs) persistently sample their surroundings by seemingly random extension and retraction of their protrusions. Quantifying these sampling dynamics over time and comparing RTM behaviour under different conditions can uncover certain patterns or strategies in RTM sampling, which will then help us to understand how RTMs ensure tissue homeostasis. In this project, we have employed a high-resolution intravital imaging protocol to generate movies of RTM sampling dynamics *in vivo*. Next we have built an image processing pipeline to assess cell dynamics via its shape, the curvature and displacement of the cell membrane as well as the movement of the cell protrusions over time. Such detailed measurements enable differentiating physiological states of RTMs, and will help to build a quantitative mathematical model for RTM protrusion dynamics.

BP 28.54 Thu 18:00 P2/EG

The energy cost of membrane-cortex deformation in phagocytosis of different sized pathogens — •Mehdi Ait Yahia and Rhoda Joy Hawkins — University of Sheffield

During their lifetime macrophages (a type of white blood cell) defend against infection in biological organisms by moving and interacting with micrometer sized pathogens. Interactions include phagocytosis which is the engulfment of pathogens by the cell deforming around the target. We model the physical description of the deformation of the membrane and cortex composition based on the energy of bending and stretching. For the bending energy we use the Helfrich energy for an elastic membrane in terms of its elastic moduli and curvature. The stretching energy is a function of the moduli and the extra surface needed to engulf the target object. We consider different methods to obtain the elastic moduli including the possibility of exocytosis modifying the surface area. The bending energy is expected to be smaller for larger objects since the curvature is inversely proportional to the radius. On the contrary the stretching energy is expected to increase for a larger object. We minimize the sum of these two energies with respect to the radius to find an optimum size for phagocytosis. We compare our theoretical predictions with data from simulations and experiments on macrophages engulfing beads of different sizes and the fungal pathogen Cryptococcus.

BP 28.55 Thu 18:00 P2/EG

We can see you think: Towards label-free imaging of action potentials — •Andrii Trelin[1], Heiko Lemcke[2], Sophie Kussauer[2], Christian Rimmbach[2], Robert David[2], and Friedemann Reinhard[1] — [1]Institute for Physics, University of Rostock — [2]Department of Cardiac Surgery, Rostock University Medical Center

The ability to directly observe neuronal communication like propagation of action potentials (AP) is crucial for the understanding of biological neural networks such as the mammalian brain. Existing methods either cannot access cells deep inside tissue (microelectrode arrays) or are not suitable for observing cells over long time periods (fluorescence). We are developing a novel method of AP imaging, based on the fact that the propagation of an AP through a neural network is accompanied by tiny movements due to various processes, including an increase of cell volume, a change of membrane tension, and others. Although movements happen on a nm scale, i.e. beyond the resolution of classical microscopy, theoretical estimates show that detection of these movements is possible by performing high-speed video recording of the cell and combining information from multiple pixels. The sensitivity can be amplified by employing a suitable optical setup, e.g. interferometric microscope. In this poster, we present the design of the experimental setup and share some of the results obtained in the project. Additionally, we will discuss the development of algorithms, capable of extracting cell movement information from high-speed videos. These include simple statistical analysis of videos, decomposition methods such as PCA, as well as machine learning approaches.

BP 28.56 Thu 18:00 P2/EG

Classifying single cells by their motion — •Anton Klimek[1], Debasmita Mondal[2], Prerna Sharma[2], and Roland Netz[1] — [1]Freie Universität Berlin, Germany — [2]Indian Institute of Science, Bangalore, India

We present a method to differentiate cells solely by their trajectories based on the generalized Langevin equation and apply it to distinguish two differently swimming types of strongly confined microalgae Chlamydomonas reinhardtii cells with an accuracy of 100 %. The model we use is suggested by the data and succeeds to describe the motion on the single cell level. By a simple fit we can extract model parameters for individual cells and subsequently perform an unbiased cluster analysis to determine the number of different cell types in the population and obtain an assignment of every cell to one of the types. Additionally, the model suggested by the data includes information on the underlying processes leading to the observed patterns of motion, which in the case of our Chlamydomonas reinhardtii data could hint towards a harmonic coupling between the cell nucleus and the flagellar propulsion apparatus. As it still remains a challenge to classify cells on the single cell level, the presented method to distinguish cells with as little information as their trajectories might have important implications in biology and medicine.

BP 28.57 Thu 18:00 P2/EG

The role of vimentin in endothelial cells under flow — •Julia Kraxner[1,2], Wolfgang Giese[1,2], and Holger Gerhardt[1,2] — [1]Integrative Vascular Biology, Max Delbrück Center for Molecular Medicine in the Helmholtz Association (MDC) — [2]German Center for Cardiovascular Research (DZHK), partnersite Berlin

Vascular endothelial cells (VECs) compose the inner layer of blood vessels where they need to be able to constantly sense, withstand and

adapt to varying mechanical stresses. For the sensing and adaptation to mechanical stress cytoskeletal proteins, i.e. actin, microtubules and intermediate filaments, play an important role. Here, we focus on vimentin which is the most abundant intermediate filament in VECs. These cells are constantly exposed to shear stress and they response to the flow by polarizing and aligning in direction of flow. We investigate the role of vimentin in this flow response by exposing VECs to shear stress in vitro. Furthermore, experiments under flow reveal an increase of specific phosphorylation sites in vimentin. We study the role of these specific phosphorylation sites on the mechanotransduction. Therefore, we want to combine traction force microscopy under flow with mutations in vimentin which inhibit phosphorylation of specific sites. Additionally, we plan on tuning the substrate stiffness to study the effect of tissue mechanics observed in aging of the vascular system and possible effects on mechanotransduction. These insights have the potential to improve our understanding of the complex mechanism of mechanotransduction in VECs.

BP 28.58 Thu 18:00 P2/EG

Optical Stretcher for Adherent Cells — •Alexander Janik, Tobias Neckernuss, and Othmar Marti — Institute of Experimental Physics, Ulm University

The characterization of cellular viscoelastic properties by utilizing the interface force arising from a laser beam shining through the cell has proven to be a valuable method for suspended cells, e.g. red blood cells.

The work presented here is based on the same phenomenon. A laser locally pulls the membrane of an adherent cell upwards, while the displacement is detected by off-axis interferometry. In proof-of-concept measurements, it is shown, that this contact-free method is sensitive enough to determine the complex shear modulus of stiff adherent NIH-3T3 cells. Laser power and wavelength are chosen to minimize heating induced softening.

BP 29: Statistical Physics of Biological Systems II (joint session BP/DY)

Time: Friday 9:30–12:00 Location: BAR Schö

BP 29.1 Fri 9:30 BAR Schö

Evolutionary optimization of multicomponent phase separation — •David Zwicker[1] and Liedewij Laan[2] — [1]MPI-DS, Göttingen, Germany — [2]TU Delft, The Netherlands

Biological cells use passive phase separation to segregate different biomolecules into various condensates. Since the molecular interactions determine the number of distinct condensates and their composition, they have likely been optimized evolutionarily for robust segregation. To study this, I will present a numerical method that efficiently determines coexisting phases in multicomponent liquids and use it in evolutionary optimization experiments. I will demonstrate that the optimized interactions lead to a precise number of different condensates, even if the overall composition varies. Consequently, adjusting microscopic interactions leads to stable emergent behaviors in these complex systems.

BP 29.2 Fri 9:45 BAR Schö

Kinetics of droplet sizes in non-conserved emulsions — •Jacqueline Janssen[1], Frank Jülicher[1], and Christoph A. Weber[2] — [1]Max Planck Institute for the Physics of Complex Systems — [2]University of Augsburg

Droplets form via phase separation and coexist with a dilute phase that is composed of droplet material of lower concentration. Many droplets in an emulsion undergo coarsening to the thermal equilibrium state that corresponds to a single droplet in a finite system. In passive emulsions, where the total amount of droplet material is conserved, the average radius grows as a function $t^{1/3}$ in time, and the droplet size distribution function broadens. Here we consider emulsions for which the total droplet material is not conserved, e.g. material is supplied by a chemical reaction or external reservoirs. We calculate the kinetics of droplet sizes and show that there is a switch from coarsening to narrowing of the size distribution upon material supply. Regulation of droplet sizes by material supply could be relevant for biomolecular condensates in living cells.

BP 29.3 Fri 10:00 BAR Schö

Dynamics of vesicle clusters studied by passive x-ray microrheology — •Titus Czajka[1], Charlotte Neuhaus[1], Jette Alfken[1], Moritz Stammer[1], Yuriy Chushkin[2], Diego Pontoni[2], Christian Hoffmann[3], Dragomir Milovanovic[3], and Tim Salditt[1] — [1]Institut for X-ray Physics, Georg-August-Universität Göttingen, Germany — [2]ESRF, Grenoble, France — [3]Laboratory of Molecular Neuroscience, DZNE, Berlin, Germany

Inferring the viscoelastic properties of a complex fluid from the dynamics of suspended tracer particles is a common method to perform rheological measurements where a direct measurement of the constituents of the system is not possible or impractical. The previously observed pool formation of vesicles induced by divalent salts or the protein synapsin I is a case in point. One would like to know how the mobility of a single (tracer) particle changes in a dense pool as compared to a homogeneous vesicle suspension. Here we used x-ray correlation spectroscopy (XPCS) to measure silica nanoparticles immersed in a complex biomolecular fluid composed of small unilamellar vesicles and $CaCl_2$, or SUVs and Synapsin-Ia protein, both in buffer solution. While the former system leads to irregular clusters, the latter has been observed to form protein induced vesicle pools, suggesting a liquid-liquid phase separation. Analysis of the photon correlation functions reveals the presence of different timescales, which we attribute to the free diffusive motion of the tracer particles and the motion of the tracer particles that interact with the cluster.

BP 29.4 Fri 10:15 BAR Schö

A stereotypical sequence of condensation and dispersal of RNA polymerase II clusters during stem cell differentiation — •Tim Klingberg[1], Irina Wachter[2], Agnieszka Pancholi[2], Roshan Prizak[2], Priya Kumar[3], Yomna Gohar[3], Marcel Sobucki[2], Elisa Kämmer[2], Süheyla Eroğlu-Kayikçi[2], Sylvia Erhardt[2], Carmelo Ferrai[3], Vasily Zaburdaev[1], and Lennart Hilbert[2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Karlsruher Institut für Technologie — [3]Universitätsmedizin Göttingen

Most eukaryotic genes are transcribed by RNA polymerase II (Pol II). In stem cells, recruited Pol II forms prominent, long-lived clusters, which gradually disappear during differentiation, so that only smaller clusters remain. Here, we ask whether the loss of large Pol II clusters is a stereotypical transition that can be explained by changes in the Pol II transcriptional state during differentiation. We assess clusters by super-resolution microscopy in three different experimental models of differentiation. In all cases, Pol II clusters first become larger and rounder, then unfold, and finally split into small clusters. These shape changes are accompanied by changes of transcriptional activity of Pol II. Previous work suggests a surface-condensate model, where enhancer regions support Pol II cluster formation, and transcriptional activity disperses clusters. Using this theoretical model, we propose that the developmental changes in enhancer marks and transcriptional activity during differentiation are sufficient to define a stereotyped trajectory through a cluster shape space.

BP 29.5 Fri 10:30 BAR Schö

Anomalous dynamics of differentiated droplets — •Xi Chen[1], Frank Jülicher[2], Jens-Uwe Sommer[1], and Tyler Harmon[1] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theory der Polymere 01069 Dsden — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden

Membraneless compartments formed by liquid-liquid phase separation in cells behave like droplets and take part in various biological processes. The function of these droplets are largely dependent on their components. We previously showed with a theoretical model that droplets can undergo a differentiation process where a homogeneous population of droplets converts into two coexisting types of droplets. We proposed this allows droplet specialization similar to cell differentiation.

These differentiated droplets exhibit new features and anomalous dynamics. Like a normal droplet system where droplets ripen and merge into one big droplet, this differentiation can significantly accelerate this

Ostwald ripening. This happens with the caveat that instead of ripening into one droplet, it ripens into two droplets of different types with a competing reverse Ostwald ripening process. Unexpectedly, these differentiated droplets divide and repel each other over long distances.

15 min. break

BP 29.6 Fri 11:00 BAR Schö

Microrheology of red blood cell cytosol — •Thomas John and Christian Wagner — Universität des Saarlandes, Saarbrücken

Tracking of small particles undergoing a Brownian motion is a widespread method in passive microrheology. Washed human red blood cells (RBC) are destroyed by ultrasound treatment to extract the cytosol, the hemoglobin and protein solution inside the cells. We use microrheology with sub-micrometer-sized particles to determine the viscosity of the cytosol. Since the cytosol is always diluted with an unknown amount of water due to the treatment, this small dilution has a huge impact on the viscosity. To circumvent this problem, we measured very accurately the mass density of every sample. However, the resulting density-viscosity relation is a strong monotonic increasing relation. In a separate experiment we determined the mass density distribution of individual intact RBCs in a continuous density gradient by centrifugation. Finally, we can present the probability density distribution of the viscosity in naturally distributed human RBCs.

BP 29.7 Fri 11:15 BAR Schö

Clonal dynamics at tissue interfaces — •Ruslan Mukhamadiarov[1,2], Matteo Ciarchi[1,2], Fabrizio Olmeda[1,2], and Steffen Rulands[1,2] — [1]Ludwig Maximilian University of Munich, München, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Tissue morphogenesis relies on the spatial separation of different cell types. Understanding how cells regulate the positions of such interfaces is key to understanding the processes that occur during dysregulation, such as in cancer. Genetic tracing has become an important experimental tool in studying the regulation of cell behaviour. However, its use in both homeostatic and growing tissues is limited by the emergence of universal size distributions. Here, we show that the mechanisms of tissues interface regulation is reflected in cell-fate specific size distributions of genetically labelled cells, termed clones. Specifically, we show how interface fluctuations affect the size distributions of labelled clones and derive theoretical predictions for a range of biologically relevant scenarios that can be tested experimentally. We test our theoretical framework by stochastic simulations and analysis of live imaging experiments. By relating interface fluctuations to clone size distributions our work paves the way for using genetic tracing experiments to understand the mechanisms underlying tissue compartmentalization.

BP 29.8 Fri 11:30 BAR Schö

Multivalent binding proteins can drive collapse and reswelling of chromatin in confinement — •Sougata Guha and Mithun K. Mitra — Department of Physics, IIT Bombay, India

Collapsed conformations of chromatin have been long suspected of being mediated by interactions with multivalent binding proteins, which can bring together distant sections of the chromatin fiber. In this study, we use Langevin dynamics simulation of a coarse grained chromatin polymer to show that the role of binding proteins can be more nuanced than previously suspected. In particular, for chromatin polymer in confinement, entropic forces can drive reswelling of collapsed chromatin with increasing binder concentrations, and this reswelling transition happens at physiologically relevant binder concentrations. Both the extent of collapse, and also of reswelling depends on the strength of confinement. We also study the kinetics of collapse and reswelling and show that both processes occur in similar timescales. We characterise this reswelling of chromatin in biologically relevant regimes and discuss the non-trivial role of multivalent binding proteins in mediating the spatial organisation of the genome.

BP 29.9 Fri 11:45 BAR Schö

A possible application of the Physics of topological defects to oncology — •Andy Manapany, Leïla Moueddenne, Sébastien Fumeron, Bertrand Berche, and Loriane Didier — Université de Lorraine

We propose a numerical study of the thermal diffusion process in non-Euclidian geometry applied to biological active matter. Thanks to the similarities displayed by both nematic and cells in biological tissue, we aim to apply results derived from the study of diffusion processes around topological defects found in liquid crystals, in order to highlight the thermal response in the vicinity of certain disclination defects found in epithelial tissues. This work is motivated by the fact that these types of disclination defects, mainly "comet" and "trefoil" systematically appear during metastatic phases in some forms of aggressive cancers. Thus, a study of the thermal footprint in such mediums may give us information on the most efficient ways to perform thermal ablation targeted towards aforementioned cells while preserving healthy surrounding tissue.

BP 30: Active Matter V (joint session BP/CPP/DY)

Time: Friday 9:30–12:00 Location: TOE 317

Invited Talk BP 30.1 Fri 9:30 TOE 317

Experiments on Active Polymer-Like Worms — •Antoine Deblais[1], Daniel Bonn[1], and Sander Woutersen[2] — [1]Van der Waals-Zeeman Institute, Institute of Physics, University of Amsterdam, 1098XH Amsterdam, The Netherlands — [2]Van't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, 1098XH Amsterdam, The Netherlands

We propose a new 'active particle' system in which the particles are in fact polymer-like: the Tubifex tubifex or 'sludge' worm. I will discuss three recent experiments that highlight the richness of this active system. In the first experiment, we perform classical rheology experiments on this entangled polymer-like system. We find that the rheology is qualitatively similar to that of usual polymers, but, quantitatively, the (tunable) activity of the particle changes the flow properties. In a second experiment, we disperse the worm in a quasi-2D aquarium and observe their spontaneous aggregation to compact, highly entangled blobs; a process similar to polymer phase separation, and for which we observe power-law growth kinetics. We find that the phase separation of active polymer-like worms occurs through active motion and coalescence of the phase domains. This leads to a fundamentally different phase-separation mechanism, that may be unique to active polymers. Finally, in the remaining time, I will briefly show that we can efficiently separate by size and activity these living polymers using hydrodynamic chromatography technics.

BP 30.2 Fri 10:00 TOE 317

Filamentous Cyanobacteria Aggregate at Light Boundaries — •Maximilian Kurjahn[1], Leila Abbaspour[1], Philip Bittihn[1], Ramin Golestanian[1,2], Benoît Mahault[1], and Stefan Karpitschka[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, OX1 3PU, Oxford, UK

Filamentous cyanobacteria are among the oldest, yet still most abundant phototrophic prokaryotes on Earth, fixing vast amounts of atmospheric carbon by photosynthesis. Gliding motility, coupled to photophobic responses (direction reversals in response to light intensity gradients), are believed to drive accumulation in suitable light conditions. Here, we demonstrate that photosensitivity goes beyond simple accumulation: Super-filamentous aggregates, capable of collective mechanical action, form at the boundaries of illuminated regions and may, for instance, contract and detach from the substrate, once grown to a critical mass. We explore how the light pattern, in particular its boundary curvature, impacts aggregation. A minimal model of active rods captures the behavior qualitatively. The ecological impact of such behavior is still unclear, but may enable colonies to escape from saturated habitats by switching to a planktonic state.

BP 30.3 Fri 10:15 TOE 317

Odd dynamics of living chiral crystals — •Tzer Han Tan[1,2,3,4], Alexander Mietke[4,5], Junang Li[4], Yuchao Chen[4],

Hugh Higinbotham[4], Peter Foster[4], Shreyas Gokhale[4], Jorn Dunkel[4], and Nikta Fakhri[4] — [1]MPI-PKS, Dresden, Germany — [2]MPI-CBG, Dresden, Germany — [3]CSBD, Dresden, Germany — [4]MIT, Cambridge, USA — [5]University of Bristol, Bristol, UK

Active crystals are highly ordered structures that emerge from the self-organization of motile objects, and have been widely studied in synthetic and bacterial active matter. Whether persistent crystalline order can emerge in groups of autonomously developing multicellular organisms is currently unknown. Here we show that swimming starfish embryos spontaneously assemble into chiral crystals that span thousands of spinning organisms and persist for tens of hours. Combining experiments, theory and simulations, we demonstrate that the formation, dynamics and dissolution of these living crystals are controlled by the hydrodynamic properties and the natural development of embryos. Remarkably, living chiral crystals exhibit self-sustained chiral oscillations as well as various unconventional deformation response behaviours recently predicted for odd elastic materials. Our results provide direct experimental evidence for how non-reciprocal interactions between autonomous multicellular components may facilitate non-equilibrium phases of chiral active matter.

BP 30.4 Fri 10:30 TOE 317

Optimal collective durotaxis through active wetting — Macià-Esteve Pallarès[1], Irina Pi-Jaumà[2], Isabela Corina Fortunato[1], Valeria Grazu[3], Manuel Gómez-González[1], Pere Roca-Cusachs[1], Jesus de la Fuente[3], •Ricard Alert[4], Raimon Sunyer[1], Jaume Casademunt[2], and Xavier Trepat[1] — [1]Institute for Bioengineering of Catalonia — [2]University of Barcelona — [3]Instituto de Nanociencia y Materiales de Argón — [4]Max Planck Institute for the Physics of Complex Systems

The directed migration of cell clusters enables morphogenesis, wound healing and collective cancer invasion. Gradients of substrate stiffness are known to direct migration of cell clusters in a process called collective durotaxis, but underlying mechanisms remain unclear. Combining theory and experiments, we reveal a connection between collective durotaxis and the wetting properties of cell clusters. Our experiments show that durotaxis is non-monotonic with substrate stiffness, being optimal at intermediate stiffness. Modeling the cell clusters as active droplets, we explain this non-monotonic durotaxis in terms of a balance between active traction, tissue contractility, and surface tension. Finally, we show that the distribution of cluster displacements has a heavy tail, with infrequent but large cellular hops that contribute to durotactic migration. Our study demonstrates a physical mechanism of collective durotaxis based on the wetting properties of active droplets.

15 min. break

BP 30.5 Fri 11:00 TOE 317

Chlamydomonas axonemes twist during the beat — •Martin Striegler[1,2], Benjamin M. Friedrich[3], Stefan Diez[1,2,3], and Veikko F. Geyer[1] — [1]B CUBE - Center for Molecular Bioengineering, TU Dresden, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany

Motile cilia are slender cell appendages that drive single cell locomotion and fluid transport across surfaces. The motility of cilia is generated by its inner core, the axoneme, which bends by the activity of dynein motor proteins. Generation of bending requires antagonistic dynein activity on opposing sides of the axoneme. How dyneins are activated antagonistically is unknown. Theoretical models propose dynein regulation by mechanical feedback, which entails structural deformations of the axoneme, but direct experimental evidence is missing. To study axonemal deformations during the beat, we purify and reactivate Chlamydomonas reinhardtii axonemes. Using defocused-high-speed-darkfield microscopy, we resolve the 3D waveforms with nanometer resolution on millisecond timescales. We find that asymmetric waveforms have a non-planar component, which is most pronounced during the recovery stroke. To generate non-planarity within the geometric constraints of the axoneme, twist is thought to be required. Using gold-nano-particles as probes attached to the outside of reactivated axonemes, we, for the first time, measure dynamic twisting deformations in reactivated axonemes. We hypothesize that these deformations are involved in controlling dynein motors generating the axonemal beat.

BP 30.6 Fri 11:15 TOE 317

Curvotaxis - the effect of curvature on cells and tissue — Lea Hppel, Jan Sischka, and •Axel Voigt — Institute of Scientific Computing, Technische Universität Dresden, Germany

How do cells respond to curvature? Does curvature has an influence on cell shape and movement? What are the consequences for collective behaviour of interacting cells in tissue? We address these questions using a multiphase field model on different curved surfaces and compare the results with experimental data on pillars, in tubes and other surfaces. The results show a significant influence of curvature and the possibility to effectively model the observed phenomena with classical models and additional curvature terms.

BP 30.7 Fri 11:30 TOE 317

Onset of Homochirality in Cell Monolayers — •Ludwig A. Hoffmann and Luca Giomi — Universiteit Leiden, Leiden, Netherlands

Chirality is a feature of many biological systems and much research has been focused on understanding the origin and implications of this property. Most famously, sugars and amino acids that are found in nature are homochiral, meaning that chiral symmetry is broken and only one of the two possible chiral states is ever observed. Perhaps less well-know, something similar is the case for certain types of cells too. They show chiral behavior and only one of the two possible chiral states is observed in nature. Understanding the origin of cellular chirality and what, if any, use or function it has in tissues and cellular dynamics is still an open problem and subject to much (recent) research. For example, cell chirality has already been shown to play an important role in drosophila morphogenesis.

BP 30.8 Fri 11:45 TOE 317

Dynamic instability of cytoplasmic compartments — •Melissa Rinaldin[1,2] and Jan Brugués[1,2] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany

Early embryos are the epitome of self-organization. Following the cell cycle oscillator, their internal structure is continuously reorganized into precise patterns at remarkable speeds. For example, the mm-sized egg of the frog Xenopus Laevis divides every 30 minutes into equally-sized cells. Physical processes such as autocatalytic growth, active transport, and reaction-diffusion can allow these embryos to keep up with fast cell cycle times, however, their understanding in early development remains largely elusive. Here, we present recent data from experiments of in vitro cytoplasmic extract obtained from frog eggs and exhibiting cell-free division. We show that the properties of the cell cycle oscillator regulate the pattern of cytoplasmic compartments. Specifically, by perturbing the oscillator, we establish that the interface of cytoplasmic compartments is unstable. We demonstrate that such instability arises from competing waves of autocatalytic microtubule growth, and can generate compartment fusion, strongly affecting the early embryonic pattern formation. Altogether, our results propose that the cell cycle oscillator plays a critical role in partitioning the cytoplasm of early embryos, keeping the dynamic instability of cytoplasmic compartments at bay.

BP 31: Cell Mechanics III

Time: Friday 10:00–12:00 Location: BAR 0106

BP 31.1 Fri 10:00 BAR 0106

Viscoelastic properties of cells under influence of drugs — •Henrik Siboni[1,2], Ivana Ruseska[1], Leonhard Grill[2], and Andreas Zimmer[1] — [1]Pharmaceutical Technology & Biopharmacy, University of Graz, Austria — [2]Single Molecule Chemistry, University of Graz, Austria

Nanoscale Drug Delivery Systems are an increasingly popular type of pharmaceutical treatment with the recent vaccines against COVID-19 being prime example. Here, we present out latest results in characterising preadipocyte cells when treated with protamine-miRNA nanoparticles. We employ Atomic Force Microscopy to perform force-indentation experiments in order to spatially resolve the elastic properties before and after drug treatment. Going further, we use force clamping and creep-relaxation in order to map the viscous properties as well. We then discuss the potential conclusions that can be drawn from this study and the pharmaceutical implications.

BP 31.2 Fri 10:15 BAR 0106

A mechano-osmotic feedback couples cell volume to the rate of cell deformation — Larisa Venkova[1,2], •Amit Singh Vishen[3], Sergio Lembo[4], Nishit Srivastava[1,2], Baptiste Duchamp[1,2], Artur Ruppel[5], Alice Williart[1,2], Stéphane Vassilopoulos[6], Alexandre Deslys[1,2], J. M. Garcia Arcos[1,2], Alba Diz-Muñoz[4], Martial Balland[5], J.-F. Joanny[3], Damien Cuvelier[1,2,6], Pierre Sens[3], and Matthieu Piel[1,2] — [1]Institut Curie, PSL, CNRS, UMR 144, Paris, France — [2]IPGG, PSL Research University, Paris, France — [3]Institut Curie, PSL, CNRS, UMR 168, Paris, France — [4]Cell Biology and Biophysics Unit, EMBL, Heidelberg, Germany — [5]Laboratoire Interdisciplinaire de Physique, Grenoble, France — [6]Sorbonne Université, Paris, France

Mechanics has been a central focus of physical biology in the past decade. In comparison, how cells manage their size is less understood. Here, we show that a parameter central to both the physics and the physiology of the cell, its volume, depends on a mechano-osmotic coupling. We found that cells change their volume depending on the rate at which they change shape, when they spontaneously spread or when they are externally deformed. Cells undergo slow deformation at constant volume, while fast deformation leads to volume loss. We propose a mechanosensitive pump and leak model to explain this phenomenon. This mechano-osmotic coupling defines a membrane tension homeostasis module constantly at work in cells, causing volume fluctuations associated with fast cell shape changes, with potential consequences on cellular physiology.

BP 31.3 Fri 10:30 BAR 0106

Viscoelastic characterization of biological cells in hyperbolic microfluidic channels — •Felix Reichel[1,2] and Jochen Guck[1,2] — [1]Max Planck Institute for the Science of Light, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

Research over the last decades revealed that single-cell mechanical properties can serve as label-free markers of cell state and function and that mechanical changes are a sign of alterations in the cell's molecular composition. This led to the development of a number of microfluidics tools to rapidly measure the deformability and also the viscoelastic properties of cells. The quantification of the stresses, that cause the deformation of the cells in these channels, is often challenging and with that the derivation of a stress-strain relation for such a system becomes complex. Here, we used hyperbolic channels to create an extensional flow field where the acting stresses can be measured using calibration particles and yield a simple relationship between acting stress and resulting cell strain. We then used the setup to measure the Young's modulus and bulk viscosity of HL60 cells and blood cells over a wide range of time scales. Drug induced changes to the cell state could be measured by a change in cell mechanical properties. Our simple setup offers a straightforward measurement of the viscoelastic properties of cells and microscale soft particles.

BP 31.4 Fri 10:45 BAR 0106

Pancreatic cancer metastasis: mechanics and adhesion — •Shruti G. Kulkarni[1], Malgorzata Lekka[2], and Manfred Radmacher[1] — [1]Institute of Biophysics, University of Bremen, Otto-Hahn Allee 1, 28359 Bremen, Germany — [2]Institute of Nuclear Physics PAN, Radzikowskiego 152 , 31-342 Krakow, Poland

We use Atomic Force Microscopy (AFM) to characterise the mechanical properties of Pancreatic ductal adenocarcinoma (PDAC) cell lines from the primary tumour site (PANC1), and from liver (CFPAC1) and lymph node (Hs766T) metastases. AFM measures forces using the optical lever system. To measure their stiffness, cells were probed using a rectangular cantilever with a three-sided pyramidal tip. Apparent Young's modulus (E) and power-law exponent (α) can be calculated from the force curves. To probe the adhesive properties of the cells, a single cell was attached to functionalised triangular tipless cantilevers, and then pressed against a confluent layer of cells. When the cell-cantilever is retracted, the contact of the attached cell with the cell layer is broken. The detachment exerts force on the cantilever, and this signal is also recorded by and characterised from the retract curve. The adhesion of cancer cells was measured with self-cells (the same cell line) as well as with endothelial cells (EA.hy926). CFPAC1 cells soften in confluent layers, and have increased cell-cell interaction with endothelial cells as compared to self-cells. Hs766t have similar stiffness as both single cells and as a confluent layer, and have higher cell-cell interaction with self-cells than with endothelial cells.

15 min. break

BP 31.5 Fri 11:15 BAR 0106

Dynamics of confined cell migration in 3D micro-dumbbells — •Stefan Stöberl[1], Johannes Flommersfeld[2], Maximilian M. Kreft[1], Chase P. Broedersz[2], and Joachim O. Rädler[1] — [1]Faculty of Physics and Center for NanoScience, Ludwig-Maximilians-University, Munich, Germany — [2]Department of Physics and Astronomy, Vrije Universiteit Amsterdam, 1081 HV Amsterdam, The Netherlands

Cell migration plays a key role in physiological processes such as wound healing, cancer metastasis and immune response. In previous work we have studied the non-linear dynamics of single cells migrating between two surface-patterned adhesion sites guided by a bridging line. Here, we study the dynamics of MDA-MB-231 cells captured in three dimensional (3D) dumbbell-like micro cavities. The structures formed by photolithography of PEG-Norbornene hydrogels provide a soft and hence deformable frame, while cells attach and migrate on a fibronectin-coated bottom. We find that the dwell time of cells before transitioning is retarded when the width of the dumbbell constriction is narrowed below 10 um. In this limit, deformation of the nucleus determines the time course of the repeated stochastic transitions. We measure the forces exerted by the nucleus parallel and perpendicular to the dumbbell channel walls using the displacement field of beads embedded near the 3D constriction. At the same time, the nuclear deformation is followed by confocal 4D imaging revealing an elongation and temporary decrease in nuclear volume during migration through confinement.

BP 31.6 Fri 11:30 BAR 0106

Geometry sensing by active flows: how the cell cortex can feel its shape — •Jonas Neipel and Frank Jülicher — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Morphogenesis often involves chemical patterns, e.g. defined by the concentration of signalling molecules, that specify the shape of a cell or tissue. The robustness of such processes with respect to perturbations can be enhanced by feedbacks where the generated shape impacts back on the formation of the chemical pattern. Here, we show that such shape sensing can result from the same forces that drive shape changes. We consider sheets of active matter, such as the cell cortex or a developing tissue layer, that behave as active fluid surfaces on long time scales. In these systems, forces drive flows within the surface that inevitably depend on the surface geometry of the surface. When molecules are advected by this flow, a pattern arises, reflecting the symmetries of the geometry. In particular, we show that viscous shear forces result in an effective friction force being proportional to the Gaussian curvature, such that patches of contractile stresses are advected towards regions of minimal Gaussian curvature. On a surface with spherical topology but elongated shape, this implies that a contractile ring such as the cytokinetic ring aligns perpendicularly to the long axis of the surface. Hence, the actomyosin cortex can drive align-

ment of the division axis with the long axis of the cell by a rotation of the entire cell, consistent with recent experiments.

BP 31.7 Fri 11:45 BAR 0106

Large area automated structural and mechanical analysis of developing cells and tissues — •Joerg Barner, Tanja Neumann, André Körnig, Dimitar R. Stamov, and Heiko Haschke — JPK BioAFM Business, Bruker Nano GmbH, Am Studio 2D, 12489 Berlin, Germany

Active forces in biological systems define the interactions between single molecules, growing cells and developing tissues. Atomic force microscopy (AFM) can be successfully applied for comprehensive nanomechanical characterization of such samples under near physiological conditions. Currently, the trend is to extend this by studying the mechanobiology of living cells while evaluating their structure and the interaction with their cell culture substrates.

We will demonstrate how cell spreading and migration in living KPG-7 fibroblasts and CHO cells, can be studied with high-speed AFM and associated with spatially resolved cytoskeletal reorganization events. We will further extend this with high-speed mechanical mapping of confluent cell layers, which in combination with optical tiling can be applied to automated analysis of large sample areas. As a tool for analyzing the complex cellular mechanobiology, we went beyond purely elastic models, and performed sine oscillations (up to 500 Hz, amplitude 5-60 nm) in Z while in contact with the surface to probe the frequency-dependent response of living fibroblasts.

BP 32: Closing Plenary Talk (joint session BP/CPP)

Time: Friday 12:15–13:00 Location: HSZ 03

Invited Talk BP 32.1 Fri 12:15 HSZ 03

The physical regulation of brain development — •Kristian Franze — IMP, FAU Erlangen-Nürnberg — Max-Planck-Zentrum für Physik und Medizin, Erlangen — PDN, University of Cambridge

The brain is our most complex organ system. Billions of neurons form an intricate network that regulates all major body functions including thought and emotions. However, the brain is not always that complex. It originally starts off as a simple epithelium, i.e., a single layer of cuboid cells. Axons, which transmit information to other cells over large distances, are only formed during embryonic development. Their immense length - up to several meters in some large animals - comes with severe logistic challenges. For example, how is transport of proteins and genetic information achieved from the nucleus, where the DNA is located, to the axon's distant end? And how does an axon growing through a crowded and dynamic environment know where to turn and where to connect? These questions have captured the imagination of neuroscientists for more than a century. However, despite tremendous progress in molecular biology and imaging technologies, many problems remain unresolved. Combining theory and experiments, we here identified how microtubules, which are polar polymers along which molecular motors transport cargo, orient uniformly along the axon to enable long-range transport, and how mechanical tissue properties regulate axon growth through the developing brain. Our results suggest that chemical and physical signals are integrated by neurons, and that their interaction is crucial for proper brain development and function.