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 active 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, Ger-

many — [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 codelivery 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 in-

ward 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 re-

actions. 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 Vacuum 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 amy-

loid 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.

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[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- Uni-

versität 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.